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Improving Chemical Education from High School to College Using a More Hands-On Approach

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IMPROVING CHEMICAL EDUCATION FROM HIGH SCHOOL TO COLLEGE USING A MORE HANDS-ON APPROACH

by

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DEDICATION

This work is dedicated to my family, without whose support it would have been impossible.

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ABSTRACT

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In this work, various alternative teaching methods and activities for chemical education are developed, presented, and evaluated. In the first study, an original hands-on activity using LEGO® blocks to model ionic chemical formulas is presented together with quantitative and qualitative data regarding its educational effectiveness. Students explore cation to anion ratios using LEGO® blocks to represent trivalent, divalent and monovalent cations and anions. High school chemistry students who participated in theLEGO® lab showed significantly higher post-test scores than other students. The secondstudy grows out of the creation of a computational lab module that is shown to significantly increase student learning in the subject of molecular orbital theory in first semester college General Chemistry. The third and final study presented is a course redesign project for college CHEM 1100, Preparation for General Chemistry. In this project the classroom is "flipped". Students watch video lectures at home, and spend class time working with peers and the instructor on problem solving activities. The results presented here are one of the first quantitative studies showing the effectiveness of "flipping the classroom". Students who were taught using the Reverse-Instruction (RI) method had significantly higher success in both the Preparation for General Chemistry course and traditionally taught General Chemistry I the following semester.

PREFACE

The chapters in this dissertation have been formatted for submission to the The Journal of Chemical Education.

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INTRODUCTION

The 2011 average Science Reasoning score for the nation, the state of Tennessee and Memphis City Schools are 20.9, 19.4 and 17.0, respectively. Under ACT's Educational Planning and Assessment System (EPAS) the indicator of likely success in college is provided in the College Readiness Benchmark which for Science Reasoning is a score of 24. (Success is defined as a 50% or higher probability of earning a B or higher in college chemistry.) [1] Based on this data, the average student in our city, state, and country is significantly ill prepared for college level chemistry.

Quality classroom and lab experiences can drastically improve student learning. A remarkable program implemented from Fall 2000 through Spring 2005 in rural areas of Southwestern Virginia (Appalachia), Southside Virginia, and inner city Richmond was the Mobile Chemistry Laboratory Project (MCL).[2] The MCL program which was supported with NSF (National Science Foundation), state, private, and university funding, addressed the lack of adequate high school chemistry laboratories and curricula. The MCL was combined with a chemistry kit program and provided materials for 58,640 student-conducted experiments to the area. A mobile van equipped with a full laboratory visited the schools regularly. The program also supplied teachers with the professional development to incorporate the experiences and materials into the classroom curriculum. The results were remarkable. Before the MCL program, students in the 19 schools performed an average 15.6 percent below state average on the chemistry SOL (the Virginia standardized test for chemistry). After three years of the program, the average among the 19 schools was 1.2 points above the state average. Great improvements were seen in the inner-city Richmond schools with large minority populations. Attendance also

improved on the days the mobile van was present. Unfortunately the program was terminated due to lack of funding. As this study shows, a more hands-on, active style of learning not only improves student learning but also student attitudes.

This research project is designed to create and implement, and then measure the effects of hands-on activities and alternative teaching methods on student learning in high school and freshman level chemistry. The first study presents a way to teach students the critical skill of writing chemical formulas using an interactive activity with LEGO blocks. The second study examines how a computational chemistry exercise can aid student learning at the freshman level. The final study presented is a course redesign project based on the concepts of "Reverse-Instruction" or "Flipping-the-Classroom". In such classrooms, the norm is inverted by interchanging the traditional roles of classroom lecture and required homework/problem solving. In all of these studies, quantitative results show that student performance can be vastly improved by rethinking how we teach in consideration of how students learn.

CHAPTER 1

A Building Block Activity in Writing Formulas of Ionic Compounds

Instructor Information

Background

As a teacher of high school chemistry I have tried various methods of teaching students to write formulas for ionic compounds. Most textbooks teach the familiar "criss-cross" method for writing chemical formula.[3] For years I have had students create ion card cut-outs as described in an article "The rainbow wheel and rainbow matrix: Two effective tools for learning ionic nomenclature."[4] The rainbow matrix is an online game that allows students to practice combining the correct ratio of cations and anions to make neutral compounds. In attempts to capture students' attention, teachers are always searching for fun ways to represent chemical concepts. Journal of Chemical Education Activity #43 entitled "LEGO® Stoichiometry,"[5] describes a lesson in limiting reagents where students use a LEGO® car kit as a way to visualize the concepts. Likewise in Activity #99, "Clip Clues: Discovering Chemical Formulas,"[6] a creative activity provides a hands-on learning experience using paper clips in writing formulas for ionic compounds. While LEGO® bricks have been used to illustrate various chemical concepts such as reaction kinetics,[7] design of advanced materials,[8,9] and simple elements and atoms for lower grade students,[10,11] this activity uses LEGO® bricks to teach ionic formulas. LEGO® bricks provide excellent representations of ions. Not only are the bricks color coded, but the valency of the ion can be represented by the number of dots on the brick. For example, a blue 1x3 brick (1 dot wide and 3 dots long) can represent cationic Al^{3+}. The oxide ion, O^{2-}, can be represented by a red 1x2 brick (1 dot wide and 2 dots long) (**Figure 1.1**). These two types of bricks can then be assembled to

make a product that helps students determine the cation-to-anion ratio in aluminum oxide and write the chemical formula (**Figure 1.2**).

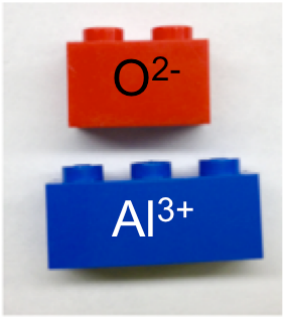


Figure 1.1. LEGO® brick "dots" represent valency of the ion. The blue 1x3 brick represents the aluminum cation with a 3+ charge. The brick is one dot wide and three dots long to represent the charge. The red 1x2 brick is one dot wide and two dots long to represent the oxide ion.

About the Activity

In this activity students build LEGO® models of ionic chemical compounds. Students may use real LEGO® bricks or virtual ones by installing LEGO® Digital Designer at

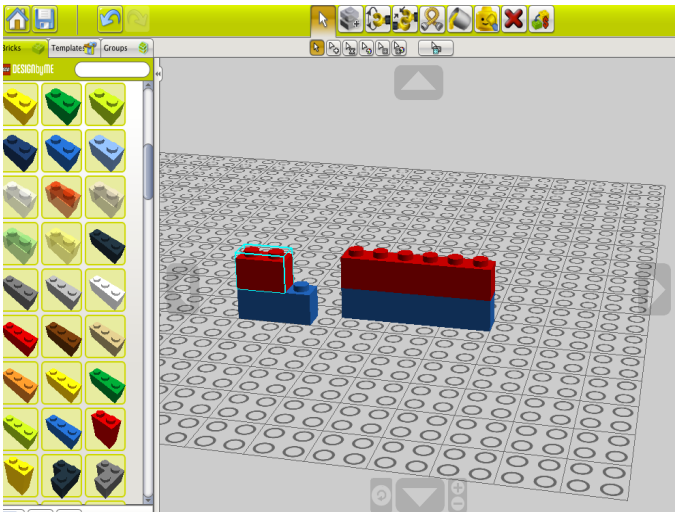


Figure 1.2. Screenshot from LEGO® Digital Designer showing model of aluminum oxide.

www.ldd.LEGO®.com. LEGO® Digital Designer is a free computer download that students can utilize to complete the entire activity (**Figure 1.2**). While in this study the students used real LEGO® bricks, I used LEGO® Digital designer over the LCD projector to introduce the activity to the class.

Students follow three rules as they build their models:

1. Trivalent, divalent and monovalent ions are represented with 1 x 3, 1 x 2, and 1 x 1 bricks, respectively.
2. Cations are blue. Anions are red.
3. Neutral formula units are rectangular using the lowest whole number ratio of bricks. All blue bricks must be placed in a single row in the final rectangular product and likewise for the red bricks.

As an example problem, students are asked to build a LEGO® model of aluminum oxide. Since Al is a trivalent cation, Al^{3+}, it is represented with a blue 1 x 3 brick. Oxide is a divalent anion, O^{2-}, and is represented with a red 1 x 2 brick. In order to create a neutral (rectangular) formula unit, we need 2 blue 1 x 3's and 3 red 1 x 2 's.

The formula is thus Al_2O_3 (**Figure 1.3).** The subscripts in the formula are determined by the number of each type of brick used. Students write the formula and the number of bricks used in a data table.

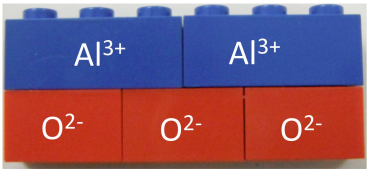


Figure 1.3. Brick model of aluminium oxide.

Integrating the Activity into the Curriculum

This activity was introduced to inner city high school chemistry students where it was used as a fun introduction to chemical formulas. As a mastery of chemical formulas is necessary for success in understanding chemical reactions, this lesson should be taught

immediately before the concepts of molar mass, balancing chemical equations and stoichiometry. A discussion of ions (monatomic and polyatomic) should precede this activity. Be sure to discuss how to deal with transition metals which need parentheses and roman numerals as illustrated by iron(II) sulfide and iron(III) sulfide. Students were directed to a table of polyatomic ions in their text. Be sure to follow-up this activity with a brief discussion of crystal lattices in order not to give the misconception that ionic structures are as simple as these LEGO® models. The students should be made to realize that these are the lowest whole number ratios of cations to anions (formula units).

Teachers can purchase enough LEGO bricks to complete this activity (12 sets) for less than $20 at the LEGO website (http://shop.lego.com/en-US/Pick-A-Brick-11998). Using this website you can choose the category “bricks” and the individual color “red” or “blue”. You can scroll down to locate 1x1, 1x2, and 1x3 bricks. Students will need three of each type of brick, (1x1, 1x2, and 1x3) both in blue and red for a total of 18 bricks per pair of lab partners. The LEGO bricks can be pre-assembled for distribution to pairs of students as shown in **Figure 1.4**. Students should be directed to return the bricks after the activity in the same fashion as they received them. The student directions instruct the

Figure 1.4. LEGO® brick set pre-assembly for easy distribution to lab partners.

students to show the teacher their model before moving on to the next model. You will want to require that they get your initials to make sure they are performing the activity correctly. With sufficient introduction and modeling by the teacher (with real bricks or using LEGO® Digital Designer and a projector) this activity requires approximately 30 minutes to complete.

Analysis of the Activity

Three separate classes in an inner-city school created three test groups. These classes were students in the same school taught by the same teacher during the 2010-2011 school year. Data were taken in the month of January 2011. One test group (the traditional group) was taught writing chemical formulas using lecture style presentation of the criss-cross method with no hands-on activities. After the lecture students were assigned group work and homework. A second test group (the virtual group) played the Rainbow Matrix game to learn how to write chemical formulas. The virtual group was also given homework. The

Table 1.1. Student Post-Test Results.

LEGO Lab	Traditional	Virtual
10	7	8
7	5	7
9	3	5
3	8	5
9	9	5
7	1	7
4	7	7
8	1	4
8	4	4
8	7	4
9	7	6
8	7	8
9	4	5
10	4	
	7	
	8	
	9	
	7	
	6	
	5	
	8	
	8	
	7	
	7	
	7	

third test group (lab group) participated in the LEGO® activity and also received the same homework assignment as the other two groups. All three groups were administered the same ten question multiple-choice post-test (see supplemental information). Post-test scores (including outliers) for all three groups are given in **Table 1. 1**.

As seen in **Figure 1.5**, the LEGO® lab group outperformed both the Traditional and the Virtual groups. A significant difference in post-test scores among the three test groups is seen using a one-way ANOVA test [$F(2,49) = 4.18$, $p = 0.021$]. Post hoc comparisons using the Tukey-Kramer test for differences between means show that the

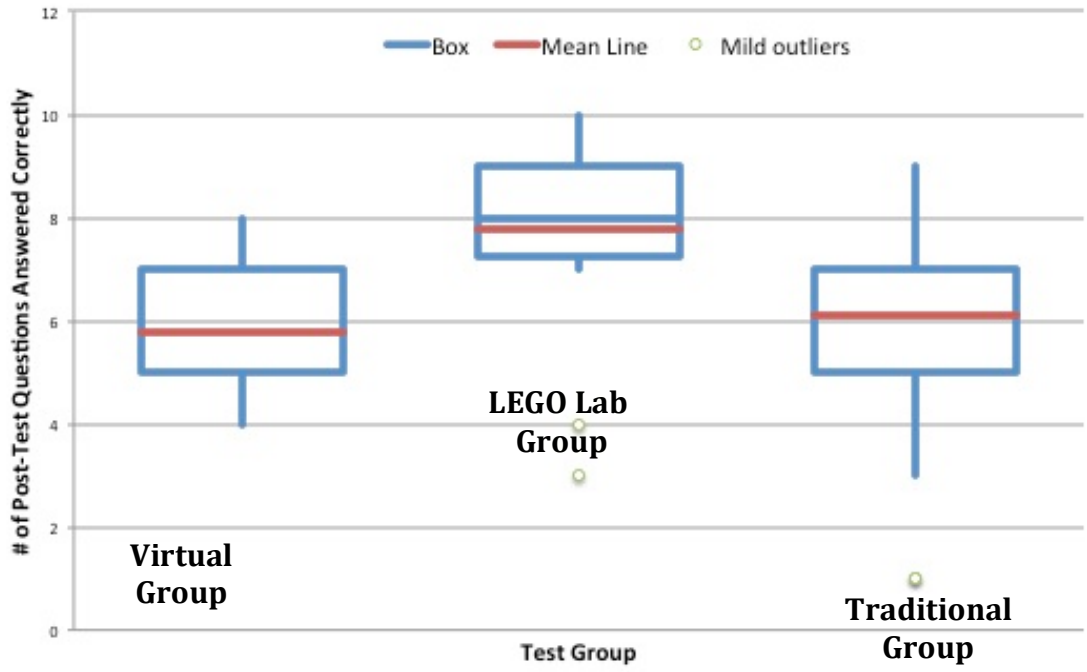


Figure 1.5. Box-plot of post-test results.

mean score for the LEGO® Lab group (M= 7.79, SD=2.04) was significantly higher than both the Traditional group (M= 6.12, SD=2.20) and the Virtual group (M=5.77,

SD=1.48). However, the Virtual and Traditional groups' mean scores did not differ significantly. Students had trouble with the Rainbow Matrix game due to unfamiliarity with the program. Student learning in the Virtual group would require more class time for students to feel comfortable using the program. Additionally, as **Figure 1.6** illustrates, the Lab group outperformed both the virtual group and the traditional group for 8 out of 10 test items. Note that the traditional group is larger in size than both other test groups, the researcher had access to these three classes and chose to assign the largest class to the traditional group due to the lecture-style nature of the activities associated with teaching the traditional criss-cross method. The traditional group could have been placed at a slight disadvantage due to its size, but note the traditional group performed comparably to the smaller virtual group. Additionally, the mean score of 7.79 for the lab group is significant even without comparison to other test groups. One reviewer pointed out that a) for question #4 (**Figure 1. 7**) includes (III) after aluminum which is technically

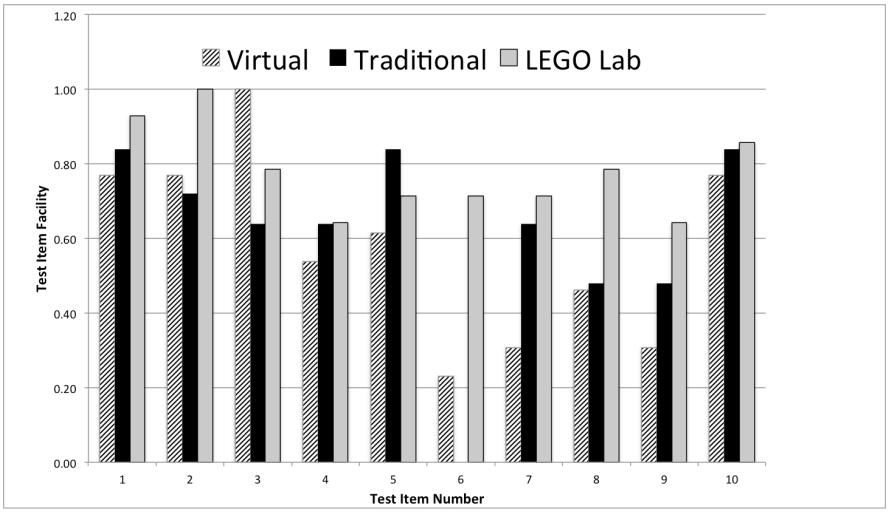


Figure 1.6. Post-test scores by item for Virtual, Traditional, and LEGO® Lab groups.

- answer (,not correct. This mistake could have resulted in the relatively low number of correct responses for this item.

In conclusion, a fun, effective, and low-cost classroom activity using LEGO bricks to model ionic formulas has been created and tested in an inner city high school classroom. Students who participated in this activity showed higher post-test scores than did students who were taught by both a traditional lecture style and using a virtual game available online.

Which of the following formulas of metal oxides is incorrect?	
a. Al_2O_3 is aluminum(III) oxide.	c. Na_2O is sodium oxide.
b. Fe_2O_3 is iron(III) oxide.	d. MgO_2 is magnesium oxide.

Figure 1.7. Question 4 on the Post-Test.

Supporting Information (See Appendix I)

Student Activity Worksheet

Student Activity Worksheet Answers

Post-test

CHAPTER 2

Introductory Molecular Orbital Theory: An Honors General Chemistry Computational Lab as Implemented in ChemBio3D Ultra 12.0

Introduction

Technological advances have made possible rich computational chemistry research programs that greatly advance the field of chemistry. User friendly interfaces for previously cumbersome computational procedures for modeling chemical systems allow computational chemistry to be utilized beyond the specialist's research laboratory. In this study, a computational module that introduces molecular orbital theory of small molecules to honors general chemistry students is presented. Tentative evaluation was performed to measure the effectiveness of the module on student learning. The software package, ChemBio3D Ultra 12.0, is part of CambridgeSoft Corporation's ChemBioOffice Ultra 2010 Suite.[12] ChemBio3D is a user-friendly modeling package from which various types of computations can be easily performed. ChemBio3D works in conjunction with the popular ChemBioDraw program used for rendering 2D molecules and reaction schemes. Since many universities and colleges already have access to this software, a computational experiment for undergraduates that utilizes this resource is particularly convenient. While computational experiments have been implemented in upper-level undergraduate organic[13] and inorganic[14] courses, few computational experiments that effectively introduce molecular orbital theory at the general chemistry level have been published with quantifiable results. Studies which introduce computational chemistry in the general chemistry classroom through the use of expensive software packages have been reported.[15,16] The most unique aspect of our computational activity is the fact that

we utilized software many schools already own, ChemBio3D. No expensive computational packages or hardware are required. We tested this module in our standard university computer lab equipped with no more than ChemBio3D which most universities and colleges use for drawing purposes only. Although there has been a trend away from the concepts of molecular orbital theory in first year college chemistry, a brief introduction such as this module could help prepare them for upper level classes where these concepts cannot be avoided. Additionally, it is imperative that students (especially Honors level students) understand that these models, be they valence bond theory or molecular orbital theory, are simply models and methods of understanding the bonding in molecules.

This computational molecular orbital theory experiment was introduced to a first semester honors general chemistry course. Students used the GAMESS[17] (General Atomic and Molecular Electronic Structure System) quantum mechanical software (as implemented in ChemBio3D) to optimize the geometry for various small molecules. Extended Hückel[18] calculations were also performed using ChemBio3D, and the results were then used to develop molecular orbital theory descriptions of the bonding. Both quantitative (post-test results) and qualitative (online student evaluations) data were utilized in the assessment of student learning.

The Module

This activity was designed as a laboratory investigation or out-of-class activity to supplement lecture material on molecular orbital theory. In particular, this module was created to help students visualize sigma and pi overlap of atomic orbitals to form molecular orbitals and to understand how atomic orbitals combine to form bonding,

antibonding, and non-bonding molecular orbitals. In the module activity (included in Supplemental Information) students investigated bonding in small diatomics (H_2, N_2, NO) and CO_3^{2-}. The concepts of bond order and spin multiplicity were introduced. Learners were guided through the creation of molecular orbital energy diagrams and were coached in the use of these diagrams to describe bonding in these small systems.

The module consists of four instructional components designed to teach students how to use computational chemistry to investigate bonding in small molecules and present the results in terms of molecular orbital diagrams. Component 1 is a pre-laboratory assignment in valence bond theory. Component 2 provides background information with an introduction to computational chemistry and molecular orbital theory. Molecular orbital diagrams of H_2 and Be_2 are discussed. Shortcomings of valence bond theory are presented. The concepts of bond order, LCAO (linear combination of atomic orbitals), bonding and antibonding combinations, geometry optimizations and the harmonic oscillator approximation are introduced. In Component 3, students explore bonding in diatomics using GAMESS[17] for geometry optimizations and Extended Hückel[18] calculations to visualize renditions of the molecular orbitals and create molecular orbital diagrams. To minimize computational expense, computations are performed at the Hartree Fock level of theory using the default 3-21G basis set. Students are introduced to closed vs. open shell calculations and spin multiplicity when they compare the optimization results for neutral H_2 vs. anionic H_2^- and neutral N_2 vs. anionic N_2^-. A dramatic visualization is the bond lengthening when electrons were added to antibonding orbitals and taken away from bonding orbitals. Students are able to see the bond length grow when an extra electron is added to the N_2 molecule and associate

this effect with the addition of an electron into an antibonding orbital. Students are able to visualize and manipulate 3D models of σ, σ*, π, and π* type molecular orbitals. Students built the NO molecule and were asked to compute its bond order. Students saw how molecular orbital theory better handles such a molecule vs. valence bond theory. As **Figure 2.1** shows, students are able to compare and contrast the molecular orbitals of homonuclear diatomics (N_2) vs. heteronuclear diatomics (CO). These images led to discussions about why the orbitals are not symmetrical in the case of CO. Students are able to call on previous knowledge of electronegativity to understand these concepts which cannot be represented in valence bond theory. Component 4 moves beyond diatomics to bonding in the carbonate ion. Students visualize π-type and σ-type molecular orbitals formed from linear combinations of atomic orbitals from all four atomic centers. Striking visualizations helped students understand the power of molecular orbital theory to handle more complex molecules where valence bond theory requires resonance structures to discuss bonding in CO_3^{2-}. After completing the four instructional components students conducted independent investigations of the bonding in CO, NH_3, and H_2O. Examples of the renditions of molecular orbitals generated by students using this module are shown in **Figure 2.1**. The shading represents the sign of the molecular orbital.

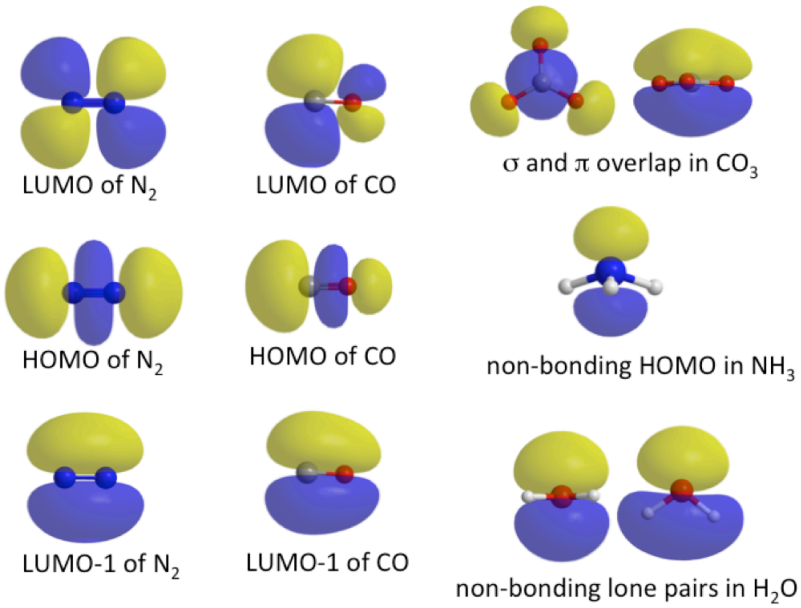


Figure 2.1. Renditions of the molecular orbitals generated using ChemBio3D.

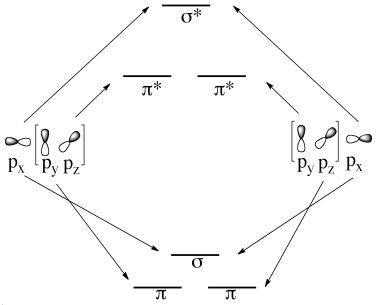
Post Test

The post test (**Figure 2.2**) was designed to measure the students' mastery of basic elements of molecular orbital theory. Students in lecture and lab are being taught about types of overlap of atomic orbitals to form molecular orbitals. Students should be able to interpret a simple molecular orbital diagram, understand the types of overlap that can result when atomic s and p orbitals combine. Students should also understand the concepts of bonding and antibonding orbitals and bond order. Students should be able to calculate bond order and predict how bond strength changes when electrons are added or

Introductory Molecular Orbital Theory Quiz

1) What type of overlap can possibly occur in the molecular orbitals formed from the combination of two p-type atomic orbitals?

a. σ and σ*
b. σ, σ*, and π
c. π and π*
d. σ, σ*, π, π*



2) Given the molecular orbital diagram, which orbitals are degenerate?

a. σ and σ*
b. the two π*
c. the two π
d. both b and c

3) What type of molecular orbitals are present in H_2 ?

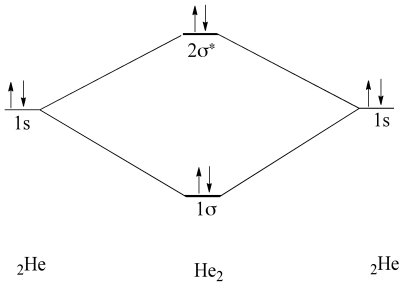
α. π antibonding
a. σ bonding
b. π bonding
c. both a and b

4) Bond order is calculated by

a. summing the number of electrons in bonding orbitals
b. (bonding electrons – antibonding electrons) * 2
c. (antibonding electrons – bonding electrons)/2
d. (bonding electrons – antibonding electrons)/2

5) Given the molecular orbital diagram to the right, calculate the bond order for He_2 .

a. 0
b. 2
c. 2.5
d. 1



6. Predict how the bond order will change upon removing an electron from He_2 to form the cation, He_2^+.

a. The bond order will remain the same.
b. The bond order will increase by 1.
c. The bond order will decrease by 0.5 .
d. The bond order will increase by 0.5 .

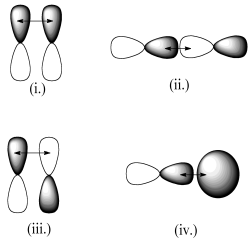
7. Which of the following will strengthen a bond between two atoms?

a. Removal of an electron from an antibonding orbital
b. Removal of an electron from a bonding orbital
c. Addition of an electron to an antibonding orbital
d. Transferring an electron from a bonding orbital to an antibonding orbital

8. A complete molecular orbital diagram is generated for a homonuclear diatomic species, X_2 . The total number of molecular orbitals is 4. Which of the following could be X_2?

a. H_2
b. He_2
c. Li_2
d. B_2

9. Which of the following types of atomic orbital overlap is BOTH sigma type and bonding (σ) ?



10. Which of the types of atomic orbital overlap in question 9 is pi (p)- type bonding overlap of p orbitals?

a. i. only
b. i. and ii. only
c. i. and iii. only
d. i., ii., and iii

Figure 2.2. Molecular Orbital Theory Post-Test

removed from molecular orbitals. All of these topics were presented in the lecture on molecular orbital theory, but the extreme visual nature of the computational laboratory aids greatly in the mastery of these concepts as will be seen in the statistical analysis to follow.

Test Groups

The students enrolled in the honors general chemistry course were divided into two groups for all laboratory experiments throughout the semester. For this experiment group 1 contained 16 students and is referred to as the module group. Group 2 contained 15 students and is referred to as the control group. The module group participated in the computational module after receiving a classroom lecture on molecular orbital theory (concurrently with the control group). The control group received only lecture material on molecular orbital theory and did not participate in the computational module.[19] Both groups were assigned the same lecture homework problems. The control group included 10 students who were participating in the Living Learning Community Program[20] offered by the University of Memphis. These students live and take core honors classes together as a part of this program and could not be separated for this study. Both groups were administered a post-test (**Figure 2.2**) on molecular orbital theory. Care was taken to ensure the control group was provided the same content (in lecture format) as the module group.

Results and Discussion.

Statistical Analysis

Post-test scores and final lecture averages for all students in both groups are presented in **Table 2.1**. **Figure 2.3** presents a box plot diagram of both the post-test scores and the

final lecture averages for the two groups. Normality tests [21] for all data show no evidence of non-normality in the post-test and lecture average data sets for both the control and module groups. Normal distribution of the data allows the F test for variances and the t-test for comparison of means to be utilized.[22] As the samples were randomly selected and the populations are normally distributed, the t-test is shown to be a robust method of comparing means between groups of small sample size.[23]

Participants in the module group reported significantly higher post-test scores (M = 7.00, var = 2.40) than participants in the control group (M = 4.73, var = 6.35), t (23) = 2.99, p = 0.01. The difference in the two means for the post-test scores is shown to be statistically significant at a 95% confidence level via a heteroscedastic t test analysis. The module group did receive three extra hours of exposure to the material by participating in the laboratory than did the control group before taking the post-test. We were pleased that the laboratory was so beneficial to student learning of such an advanced concept.

To investigate whether or not the non-randomization of the groups (as a result of the Living Learning Community group in the control) affected the results, final lecture averages are scrutinized statistically. The mean lecture averages for the control and module group are 72.65 and 74.76, respectively. No statistical difference exists between mean lecture averages for the module (M = 74.76, var = 111.50) and the control group (M = 72.65, var = 178.60), t(29) = 2.05, p = 0.63. A Pearson product-moment correlation coefficient was computed to assess the relationship between the post-test scores and the final lecture averages. A significant correlation exists at the 95% confidence level between the two variables for the module group (r = 0.73, n =16, p = 0.0015). No

correlation exists between the two variables for the control group (r = 0.20, n =15, p = 0.47) perhaps due to guessing on the post test by the control group.

Table 2.1. Post-test scores and final averages for test groups.

Student #	Control Group Test Group	Control Group Final Lecture Average	Control Group Post-Test Score (max 10)	Module Group Test Group	Module Group Final Lecture Average	Module Group Post-Test Score (max 10)
1	Control	79	0	Module	56	5
2	Control	62	2	Module	69	5
3	Control	76	2	Module	76	5
4	Control	61	4	Module	67	5
5	Control	92	4	Module	79	6
6	Control	60	4	Module	62	6
7	Control	75	4	Module	76	7
8	Control	81	4	Module	62	7
9	Control	58	4	Module	70	7
10	Control	58	5	Module	84	8
11	Control	55	5	Module	73	8
12	Control	82	6	Module	76	8
13	Control	98	7	Module	88	8
14	Control	83	9	Module	77	8
15	Control	71	10	Module	91	9
16				Module	91	10

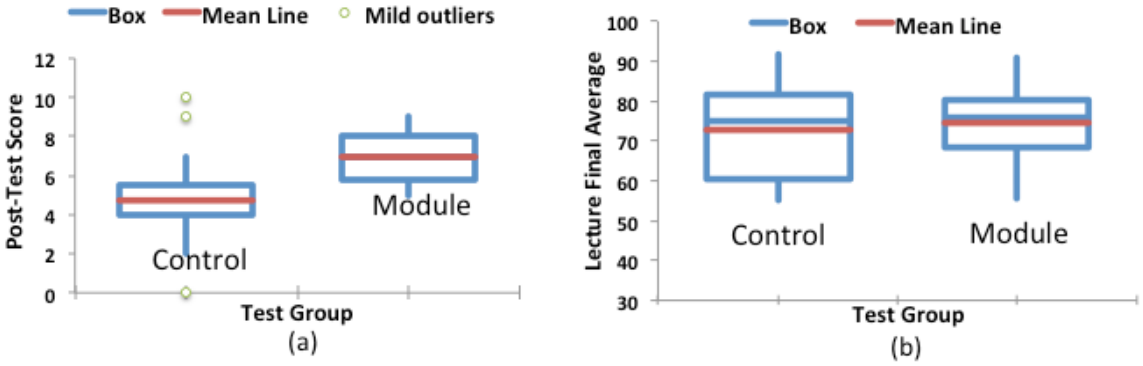


Figure 2.3. Box Plot Diagrams of (a) Post Test Scores and (b) Lecture Averages

The proportion of correct responses, or the test item facility (IF), for each of the ten multiple choice items is presented in **Figure 2.4**. The module group outperformed the control group on all items with the exception of Item 8. IF values for Item 1 are 0.69 for the module group and 0.27 for the control group. A primary goal of this module is to help students visualize concepts in 3D that can be abstract otherwise. Throughout the module students can visualize how atomic orbitals overlap in different ways to create molecular orbitals. This module effectively helps students understand the difference between s and p-type atomic orbitals and molecular orbitals formed from σ- or π-type overlap. Greater IF values for the module group on Item 1 show the efficiency of the module to help students master this concept.

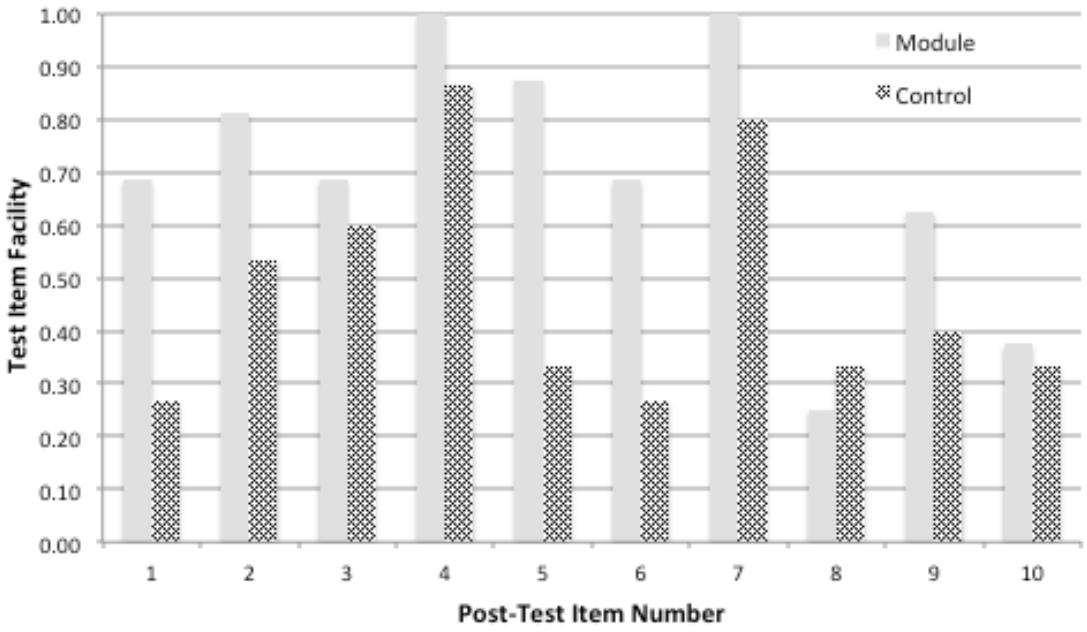


Figure 2.4. Test Item Facility (Fraction of students correctly answering an item) for Post-Test

Post test Items 4 and 5 were designed specifically to test the effectiveness of the module on stimulating higher-order thinking. Item 4 requires only the lowest level of Bloom's Taxonomy, knowledge, by testing whether the student has memorized the formula for computation of bond order. Item 5 requires a higher level of thinking, application, by requiring that students apply the formula from Item 4. While the IF values for Items 4 and 5 are high for the module group, only the IF value of Item 4 is acceptable for the control group (IF value = 0.87). Item 5 has a low IF value in the control group of 0.33 (compared to 0.88 in the module group) suggesting that completion of this module increases the students' ability to apply knowledge..

Both groups scored low IF values for Item 8 (module = 0.25, control = 0.33). In order to improve the post-test reliability for future use, Item 8 should be replaced in the post-test with a different item. Item 8 is a different type of item than any presented in the module or the lecture. In Item 8, students must decide which of four homonuclear diatomics would result in a molecular orbital diagram containing exactly four molecular orbitals. While the intended answer was Li_2, a clearer way to ask this question would be "A complete molecular orbital diagram is generated for a homonuclear species, X_2. The total number of filled molecular orbitals (core and valence shell) generated is three. Which of the following would be X_2?"

Student Assessment Survey Results

An online survey was conducted using the SALG (Student Assessment of Learning Gains) assessment tool.[24] SALG is a free course-evaluation tool that allows instructors to easily gather online learning-focused feedback from students. Originally developed in 1997[25] to assess student learning regarding modular chemistry activities, the

tool has been revised and updated to be useful in most university level classrooms. The SALG instrument focuses on how a course has enabled student learning. Students are asked to assess their own learning and the degree to which specific aspects of the course have contributed to that learning. For this study, the SALG instrument has been modified to apply to the computational MO theory module only. Complete SALG evaluation data are included in the supplemental information. Twenty-five of 31 students (module students and control students after they completed the module) participated in the SALG. Students were asked to evaluate their gains in learning based on a scale from 1 to 5 (according to the scale, 1= no gains, 2= a little gain, 3= moderate gain, 4= good gain and 5= great gain). On average students ranking values were 2.52, indicating students perceived their overall gains to be between 2: a little gain and 3: moderate gain. The highest and lowest average values are given in **Table 2.2**. Students gave highest rankings (suggesting they felt they made good gain) to Item 2.5, calculation of bond order. Lowest rankings were given to the pre-lab questions, enthusiasm generated for computational chemistry and interest in taking further chemistry classes. Low rankings for the pre-lab could have stemmed from the fact that half of the class had not yet completed the laboratory on valence bond theory before completing the module.

A complete list of all student comments is given in the Supplemental Information. The greatest percentage of positive comments (40% positive) was given to Item 1.4: "Please comment on how your understanding of molecular orbital theory has changed as a result of this experiment." An example of a positive comment provided is, "The visualization and hands on approach allowed more face-to-face time with the material."

Table 2.2. Lowest and Highest Average SALG Rankings for the MO Module.

Item	Average Response Values
Average Rankings Greater than 3.00	
2.5 Calculation of bond order	3.93
10.3 Working with peers outside of class (e.g., study groups)	3.12
1.3.2 The usefulness of Molecular Orbital Theory in the description of bonding	3.03
10.1 Interacting with the lab instructor during class	3.03
Average Rankings Less than 2.00	
6.2.1 Pre-lab assignment	1.93
7.1.1 Pre-lab questions	1.83
3.1 Enthusiasm for computational chemistry	1.73
3.2 Interest in taking or planning to take additional chemistry classes	1.73

The second highest percentage of positive responses is associated with Item 6.3: "Please comment on how the class activities helped your learning." One constructive comment was:

> "Doing the lab report and ChemBio3D module was most helpful, as it really made us articulate the difference between valence theory and MO theory and make the connection using the molecules built in ChemBio3D. Although we were given an introduction to MO theory in lecture, it would have been more helpful to have a full class dedicated to it, including talk of the energy diagrams."

Negative comments are mostly associated with Item 3.5 where students are asked to comment on how this class has changed their attitudes toward the subject of molecular orbital theory. One student responds, "I feel that the pace we moved at was too rapid for

a student who lacks prior knowledge on MOT." Many comments indicate that students felt the material was too rushed, suggesting improvements could be made by spending more time introducing the module in lecture class. As a result of this feedback, plans are being made to create an instructional video that will be included as a pre-lab exercise in the future. Students who have had more of an introduction to molecular orbital theory, and been introduced ahead of time to the module may feel less bombarded by such a new idea.

Conclusion

This computational module in molecular orbital theory enhanced student learning. We were able to use a software package already licensed by our University to introduce honors general chemistry students to both molecular orbital theory and computational chemistry. Students who participated in the module in addition to attending a class lecture scored 22.7% higher on a 10 item multiple-choice post-test than students who attended lecture alone. The post-test adequately assessed learning for the control group, but proved too easy for the module students. While the test groups were small, the t-test analysis is designed for such situations. The authors believe that the effectiveness, low cost, and ease of administration of this experiment make it a valuable tool for chemistry teachers especially those at departments who already own ChemBio 3D Ultra.

Acknowledgement

The authors thank the NASA Harriett G. Jenkins Pre-doctoral Fellowship Program for tuition and stipend support (KRR). Special thanks to Jennifer L. Petersen for help with the statistical analysis.

Supporting Information Available (See Appendix II):

1. Lab manual document

2. Lab manual answer key document

3. Revised module post-test with answers

4. Student online evaluation feedback document

CHAPTER 3

Reverse Instruction (RI) Applied to CHEM 1100, Preparation for General Chemistry: A Course Redesign Project

Introduction and Background

The 2011 national average for the Science Reasoning portion of the ACT (American College Testing) exam is 20.9 with the percent of recent high school graduates who took the ACT and scored at or below 20.9 being approximately 55%. Under ACT's Educational Planning and Assessment System (EPAS) the indicator of likely success in college is provided in the College Readiness Benchmark which for Science Reasoning is a score of 24. (Success is defined as a 50% or higher probability of earning a B or higher in the college chemistry.)[26] Based on this data, the average student in our country is significantly ill-prepared for college level chemistry. Not surprisingly, Universities must meet the needs and remediate ill-prepared students. The Department of Chemistry at The University of Memphis has received support to alter the design of our preparatory chemistry course, CHEM 1100. An all-time high number of 412 students enrolled in CHEM 1100, *Preparation for General Chemistry* during the 2010-2011 academic year. Only 143 of these students passed with grades of A, B, or C, a dismal "success" rate of 35%. In addition, the average percent success rate for CHEM 1110 (General Chemistry I) was only 41.2% during the Fall 2010 and Spring 2011 semesters. We have therefore instituted a course redesign project based on the concepts of "Reverse-Instruction" or "Flipping-the-Classroom". In such classrooms, the norm is inverted by interchanging the traditional roles of classroom lecture and required homework/problem solving. Each class meeting has been changed to emphasize hands-on learning and teaming, resulting in the conversion of the classroom to a collaborative problem-solving laboratory. Here

students receive individualized assistance (from faculty or peers) in working on problem solving by tackling online graded assignments during class time. In this way we can promote individual and small group questions that can be addressed with immediate feedback. According to recently published data[27], online homework can make a significant improvement in chemistry course retention rates and attitudes of students regarding chemistry courses. In one study quizzes were directly replaced by online homework and a statistically significant improvement ($p < .0005$) in success rates in second-term general chemistry was seen. Results also indicated that 90% of students completed the online homework and viewed the assignments as worth the effort (83.5%).[28] Attendance was mandatory and the classroom remained the site for quizzes and exams.

Reverse-instruction is being implemented in other classrooms with great success[29,30] The most attention lately has focused on the work of Salman Khan of the Khan Academy[31]. Khan and his team have created and provide free access to over 3100 academic lecture videos which have and can be used by teachers to "flip" their classroom. In Khan's webcast talk at TED in 2011 he points to some feedback from youtube.com comments where students mention that they actually prefer the videos. One great advantage to the video vs. traditional lecture is the ability to pause and rewind the lectures as much as you need. Since classroom time is not spent passively listening to lectures, Khan points out that this approach actually has "used technology to humanize the classroom." Salman Kahn was not the inventor of this idea of flipping the classroom however. In a winter 2000 article in the *Journal of Economic Education*[32] Lage and coworkers describe the results of "Inverting the Classroom" on an introductory college

economics course. The authors point out how this method of teaching is able to span the different learning styles of students. The recorded lectures are available for those students who learn best from the traditional methods, but with class time free to have discussions, work problems, do projects, and work with peers, students who benefit more from other learning styles have more of a chance for success. Reports of other classes being inverted range from an Advanced Placement Calculus AB high school class[33] to college level physics courses[34]. In 2009, Zappe and co-workers[35] flipped a large undergraduate architectural engineering course. While the results of this study are mainly derived from student evaluations of the course, in general, the classroom flip had a positive impact on student learning. Students perceived the method of teaching as more effective than lecturing, and reported that they enjoyed the class and benefited from watching the lecture videos outside of class. As a result of this study, the authors make some suggestions for effective "flipping" of the classroom. Among the suggestions are the following; 1) Students must take a video quiz to ensure they have prepared for class 2) Videos should be kept under 20 minutes. 3) Sometimes an in-class review of video material is necessary. This advice was considered in the implementation of our CHEM 1100 flipped course at The University of Memphis.

Methodology

The course redesign project was first implemented in the Fall of 2011 to CHEM 1100, *Preparation for General Chemistry*. During the Fall 2011 an advanced graduate student initiated the project as part of her Ph.D. dissertation in chemical education. She taught three sections of CHEM 1100. One of her three sections of approximately 50 students was taught using standard (ST) lecture style methodology. Her two other

sections of 25 students participated in the "flipped" classroom learning style, also known as Reverse-Instruction (RI). During the summer, 2011, thirty-two video lectures were created using Camtasia software to create videos which are voiced-over Microsoft PowerPoint lectures and example problems. The average video length is about 15 minutes. Three other lecture-based sections beginning with approximately 50 students were taught by university faculty members. The Reverse-Instruction (RI) sections watched videos of lectures outside of class and participated in working online homework problems during class with the assistance of the instructor. Working with partners was encouraged during class time. The instructor closely monitored the students' work during class, interacting with each student daily. The grading system for the graduate student's RI and lecture section was as follows: Online Homework/Classwork: 20%, Quizzes; 30%, Tests :40%, Final Exam: 10%. All sections were required to do online homework assignments, take quizzes, tests, and a common final exam created by an experienced instructor who was not currently teaching in the course. All students in the graduate student's three sections had access to videos, syllabi, PowerPoint presentations, quizzes, and other materials through their university eCourseware accounts. This project was continued into the Spring 2012 semester with the graduate student teaching two RI sections. Faculty members taught the other three sections of lecture-based classes.

The Spring 2012 RI courses were taught with the same supporting videos as used in the Fall 2011. In an attempt to make the course more effective, a few changes were made as a result of observations and evaluation of student feedback. It became obvious that some students were not consistently watching the videos. Online video quizzes were given throughout the spring semester to further motivate students to interact with the

material before coming to class. Additionally, in the fall 2011 it was noted that many students worked alone in silence, mostly guessing on many of the homework problems. In the spring 2012, online assignments were divided into two categories: classwork and homework. The classwork was a specially chosen set of problems designed to be finished in class. Students were required to work on the classwork assignments with a partner, and ask questions if they got down to their final attempt to get the problem correct. Classwork could only be completed in class. Students were closely monitored by the instructor to make sure they were on-task and working together during class. Longer homework assignments were given for each topic and made due the night before the next class. Additionally, in the Fall 2011 students had six attempts to answer online homework questions correctly. This excessive number of attempts encouraged guessing. The Spring 2012 number of attempts were limited to three for classwork and four for homework. Tests as well as quizzes were administered online providing instant feedback to the students.

Our main goal of this project is to increase our "percent success" rates in CHEM 1100 and thus increase our success rates in the subsequent CHEM 1110, *General Chemistry I,* and eventually empower more students to be successful in upper division science classes.

Results

During the first semester of implementation (Fall 2011) the two RI sections (A and B) were compared to the graduate student's lecture-based section (ST-A), and the other three lecture-based sections (ST-B, ST-C, and ST-D) that were taught by faculty members experienced in teaching this course. Mean ACT scores for all of the sections of

CHEM 1100 in this study are given in Table 3.1. These ACT scores are not statistically different, indicating that all classes began the semester at the same academic level. Quantitative evaluation of the course redesign was completed by comparing the common final exam scores and "percent success" (the percentage of students who finished the course with a letter grade of C or higher) between the RI and regular lecture sections. Additionally, student feedback was gathered using two surveys, a SALG[36] survey (*vide infra*) and The University of Memphis course evaluation system, SETE (student evaluation of teacher effectiveness).

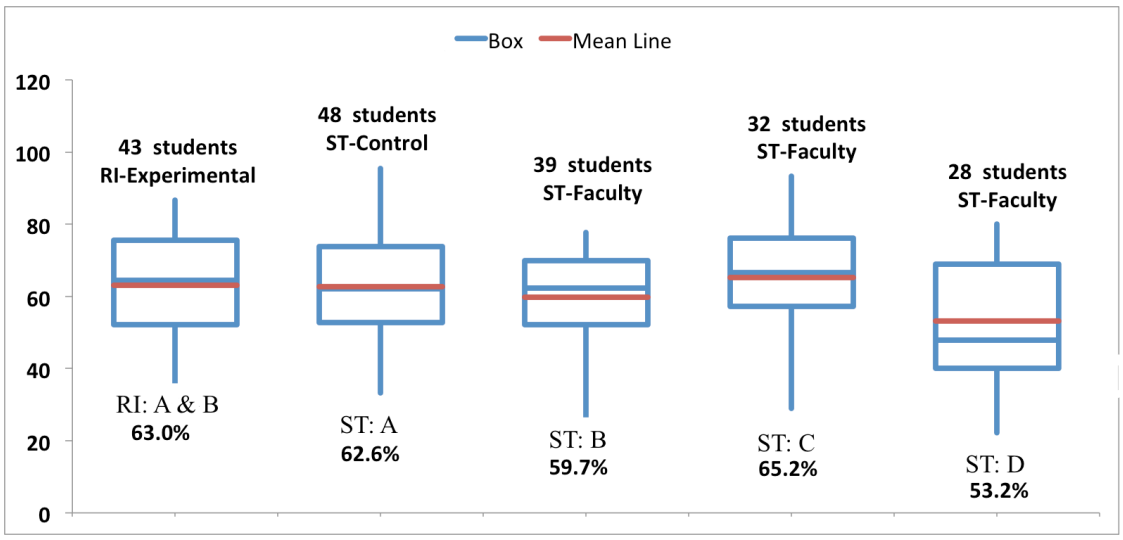
Table 3.1 Mean composite and math ACT test scores for CHEM 1100 students by section.

Fall 2011			Spring 2012		
Section	**Composite**	**Math**	**Section**	**Composite**	**Math**
RI-A	22.7	21.4	RI-A	19.3	20.3
RI-B	20.5	19.7	RI-B	20.0	20.9
ST-A	22.7	22.7	ST-A	19.2	20.5
ST-B	21.2	20.1	ST-B	20.1	21.4
ST-C	22.2	21.4	ST-C	19.4	21.1
ST-D	21.3	19.4			
MEAN	21.8	20.8	MEAN	19.6	20.8

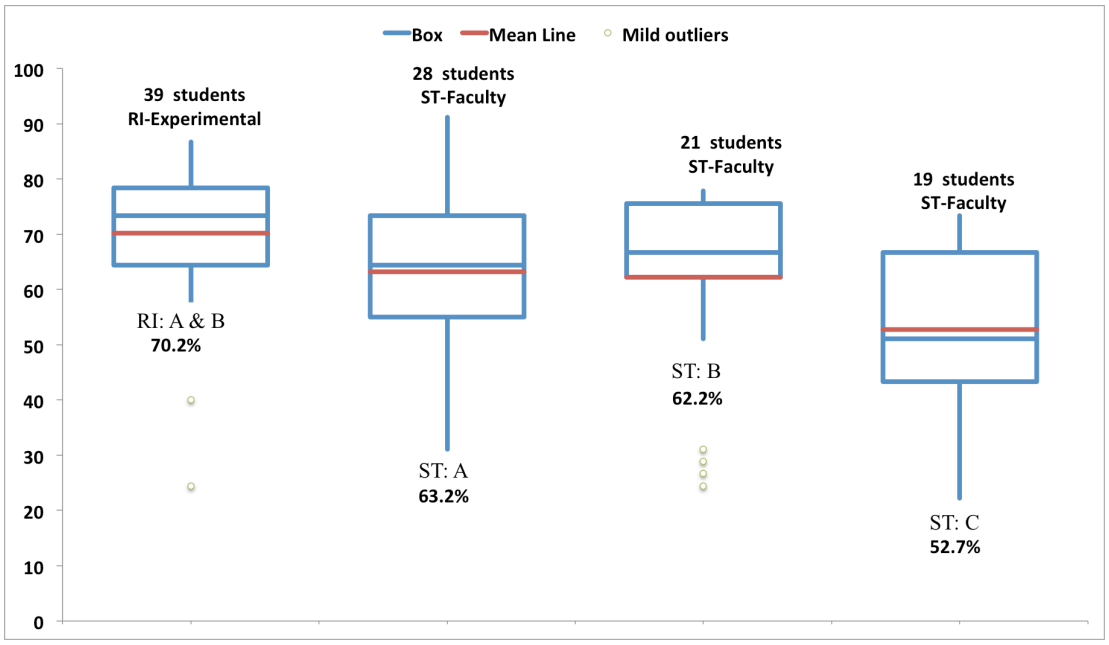
Final exam scores for all six Fall 2011 sections of CHEM 1100 are presented in **Figure 3.1(a)**. The two RI sections (A & B) are grouped together for presentation of these results. A significant difference (mainly attributable to the low performance of section ST-D) in final exam scores among the five Fall test groups is seen using a one-

way ANOVA test [$F(4,185) = 2.77$, $p = 0.028$]. *Post hoc* comparisons using the Scheffe contrasts among pairs of means show that the mean score for section ST-D was significantly lower than the other five sections (See appendix III, Table III.1). The mean scores for all other sections are not significantly different. Final exam scores (the same final exam as Fall 2011) for all five Spring 2012 sections of CHEM 1100 are presented in **Figure 3.1(b)**. The two Spring RI sections (A & B) are grouped together for presentation of these results. A significant difference (mainly attributable to the high performance of the RI sections) in final exam scores among the four test groups is seen using a one-way ANOVA test [$F(3,104) = 5.57$, $p = 0.014$]. *Post hoc* comparisons using the Scheffe contrasts among pairs of means show that the mean score for section ST-C was significantly lower than the RI sections combined (See appendix III, Table 2).

While the mean final exam scores for the RI sections were not significantly different from the lecture sections, it is important to note that the percent success rate (percent of students completing the course with a C or higher) for the RI classes was higher than all of the lecture sections (**Figure 3.2**). The contribution of student retention to the percent success rate is great. As **Figure 3.2** indicates the percent success rates are highest in the classes where a high percentage of students attended until the end of the course. The Reverse-Instruction sections are in general significantly better at retaining students throughout the semester. Not only are the average common final exam scores higher for the Reverse-Instruction (RI) classes, but the Percent Success Rate for the RI classes is much higher than that of the standard (ST) traditional lecture classes.



(a) Fall 2011 final exam scores



(b) Spring 2012 final exam scores

Figure 3.1. Box-plot diagram showing mean final exam scores for (a) Fall 2011 sections. (Reverse-Instruction sections A and B are combined. Section ST-A is a lecture based class taught by the RI graduate student. Sections ST-B, ST-C, and ST-D were taught by University faculty.) (b) Spring 2012 sections. (Reverse-Instruction sections A & B are combined. Sections ST-A, ST-B, and ST-C were lecture sections taught by University faculty.)

Note that lecture section ST-A-Fall had a much higher percent success rate than did all other ST-lecture sections. This class was the lecture section taught by the same graduate student who taught the RI sections, and this lecture section had full access to all videos and PowerPoint materials available to the RI sections. Many of the ST-A-Fall lecture students reported viewing the online videos, and most students downloaded the PowerPoint lectures before attending class. This access to extra support materials may explain why this section performed higher than the other lecture sections.

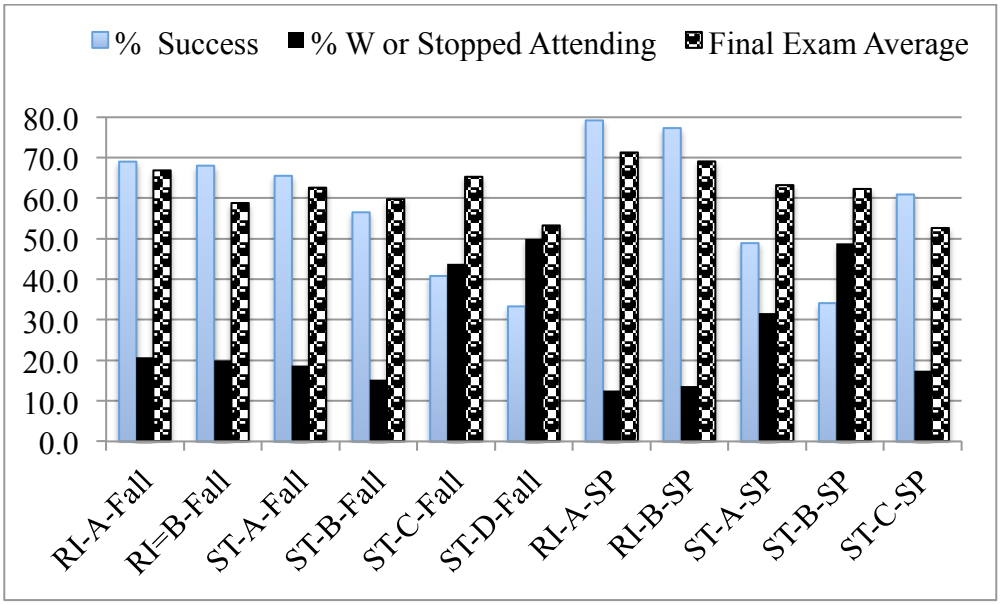


Figure 3.2. Percent Success Rates, Percent Withdrawn or Stopped Attending, and Final Exam Average for all sections of CHEM 1100 for the Fall 2011 and Spring 2012 semesters. Section ST-A-Fall(Lecture) and all RI sections were taught by the same graduate student. Remaining sections were lecture (ST) classes taught by University faculty.

Additionally, the percent success rates increased for the RI sections from the Fall 2011 (63.0% on average) to the Spring 2012 RI sections (70.2% on average). Reverse-Instruction students in the Spring 2012 sections scored significantly higher final exam scores ($M = 70.2$, var = 184) than Fall 2011 group ($M = 63.0$, var = 220), $t(81) = 1.99$, $p = 0.024$. The difference in the two means for the final exam scores is shown to be statistically significant at a 95% confidence level *via* a heteroscedastic t test analysis. This increase indicates that the course adjustments made from the Fall to the Spring were beneficial to student learning in the Reversed classroom.

Since an important goal of this project is to lay the foundation to increase the success rate in General Chemistry I (CHEM 1110), the Fall 2011 CHEM 1100 students were followed as they took CHEM 1110. The percentage of CHEM 1100 students who went on to be successful in CHEM 1110 in the Spring 2012 is shown in **Figure 3.3**. Impressively, 73.7 % of Reverse-Instruction students who completed Preparatory Chemistry and went on to take General Chemistry I were successful. Only 48.4% of students in the Lecture-Based CHEM 1100 classes were successful in General Chemistry I. These results are particularly significant since the percent success rate for CHEM 1110 (all students who took General Chemistry I) is only 52.5 %. Note the students in the graduate student's ST-A-Fall lecture based course did better than the other ST lecture-based sections, suggesting there could be some teacher influence on these data. However, the RI students still outperformed ST-A-Fall by greater than 10%.

An online survey was conducted using the SALG (Student Assessment of Learning Gains) assessment tool. SALG is a free course-evaluation tool that allows instructors to easily gather online learning-focused feedback from students. Originally

developed in 1997[37] to assess student learning from modular chemistry activities, the tool has been revised and updated to be useful in most university level classrooms. The SALG instrument focuses on how a course has enabled student learning. Students are asked to assess their own learning and the degree to which specific aspects of the course have contributed to that learning. In comparison, the university's SETE evaluations focus more on the rating of teacher than perceived learning or gains made by students. SETE evaluation results for Fall 2011 are included in the supplementary information (Appendix 3). Overall, standard lecture section ST-A, which was taught by the same graduate

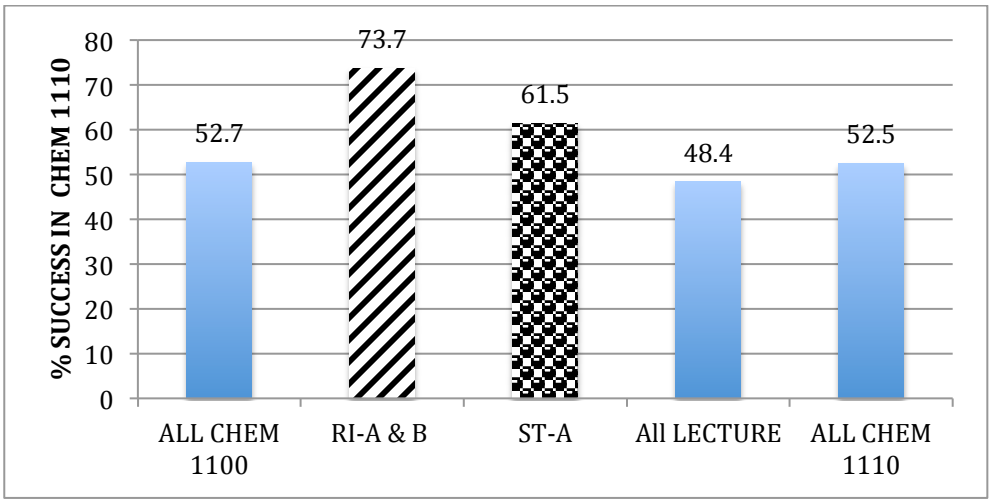


Figure 3.3. Percent of Fall CHEM 1100 students who enrolled in and successfully completed CHEM 1110 (General Chemistry I) in the Spring 2012. RI students are those who were enrolled in the Reverse-Instruction CHEM 1100. ST-A students were enrolled in the same instructors class as a standard lecture style class. All LECTURE students are all CHEM 1100 students who were taught using the standard lecture style. All CHEM 1110 students are ALL students who took General Chemistry I, regardless of whether or not they took CHEM 1100.

student who taught the two reverse-instruction sections, was ranked higher on average than all other sections. The two RI sections (A & B), received lower evaluations than the ST sections B and C. Complete SALG evaluation results are presented in the supplemental information (appendix 3) and some representative comments are provided in **Table 3.3**. Overall, the Fall 2011 traditional-lecture section gave a higher average SALG ranking of 3.73 than did the Fall 2011 reverse-instruction sections combined (3.56). The spring 2012 RI sections gave a higher overall SALG ranking than all of the Fall 2011 sections with an average ranking of 3.92. A significant difference in mean rankings among the three groups is seen using a one-way ANOVA test [$F(2,108) = 10.56$, $p = 0.0006$]. *Post hoc* comparisons using the Scheffe contrasts among pairs of means show that the mean score for Spring RI group is significantly higher ($M= 3.92$, $SD=0.24$, $p =0.00006$) than both other groups (See appendix III, Table 2). The mean scores for all other sections are not significantly different, but the p-values are low.

Some particularly insightful student comments from the Spring 2012 SALG were as follows:

- "I have been able to remember what I learned in high school and learn more about Chemistry and this material helped me understand it very easily"
- "I knew absolutely nothing about chemistry before taking Dr. Ruddick's class. I had a horrible chemistry teacher in high school so I disliked the subject. But Ruddick opened my eyes to the entertainment of chemistry. "
- "This class has made me appreciate chemistry more and I look forward to tak[ing] chemistry 1 and chemistry 2 later."
- "It made me more interested in chemistry"
- "I didn't think chemistry would ever be fun or interesting. But it is. Probably the most interesting subject. "
- "Chemistry is not so scary to me now."

- "I love the online material. Tremendously effective and helpful"
- "I like the computer assignments really helped"
- "The subject was very well organized so I didn't have any problem trying to keep up or understand unless I didn't study on my own."
- "Being able to refer back to the text and videos for help is great. That way you can receive a better understanding."
- "Like the videos and PowerPoint"

Conclusions

Our main goal of increasing percent success rates in CHEM 1100 has been achieved with the Reverse-Instruction students out-performing the standard lecture-based students with higher final exam scores and overall success in the class. The Reverse-Instruction classes have much higher retention rates than the standard lecture-based courses. As a result of this project, CHEM 1100 percent success rates improved from 35% to 78%. It is obvious from the percent success rates and student evaluation comments that students enjoyed the class and some even found a love for chemistry. This successful experience in CHEM 1100 transferred to a successful experience in traditional lecture-based General Chemistry I where 73.7% of RI students who went on to take CHEM 1110 were successful versus 48.4% from the CHEM 1100 ST (Standard Lecture-Based) classes. Additionally, the Reverse-Instruction model works best if you:

1. Prepare succinct entertaining videos.
2. Administer daily video quizzes at the beginning of class.
3. Require that students work together.

4. Encourage students to ask questions.
5. Closely monitor the class as they complete well-designed classroom activities.

This redesigned course as taught required a smaller class size and use of a computer lab. We acknowledge that the delivery of the Reverse-Instruction model may be more expensive than the larger standard lecture course. However, larger class sizes could be successful with the aide of teaching assistants to help monitor the classroom activities. Additionally, as we move toward the use of laptop computers and mobile devices in our classrooms, the need to meet the class in a computer lab will no longer exist.

Acknowledgement

The authors thank the NASA Harriett G. Jenkins Pre-doctoral Fellowship Program for tuition and stipend support (KRR).

Supporting Information Available (See Appendix III):

1. *Post hoc* analysis results for comparison of the common final exam scores.
2. Student online evaluation feedback document

CONCLUSION

In a 2010 review article entitled "What do we know about explanations for drop out/opt out among young people from STM (Science, Technology, and Mathematics) higher education programmes?" the authors presented some eye-opening findings that we as educators should not ignore.[38] The authors conclude after an extensive review of the literature and available data that "if STM programs and institutions genuinely wish to increase the number of students completing the STM programme they enter, these programs need to turn their focus from the students alone and on to themselves and the culture and values that are revered there, and consider whether they are perhaps a part of the problem." We are particularly challenged in Memphis as we mainly serve a population of students who have attended high minority schools. In the Memphis City Schools (a system serving over 100,000 students) the majority of high schools are greater than 80% minority and economically disadvantaged, with only one high school being populated by less than 61% minority students. Indeed most of our students are first-generation college undergraduates. In a 2005 study Pascarella and co-workers concluded that students whose parents have completed an undergraduate degree are more likely to successfully complete a bachelor degree.[38] Most importantly, research suggests that first-generation undergraduates are greatly affected by classroom activities compared to students with highly educated parents.[39] In light of these findings it is imperative that we at the university attempt to change in ways that will best serve our population of students. Since we have no control over the poverty rates or personal backgrounds of our incoming students then we must attempt to design programs which will provide quality educational experiences for not only the well-prepared students, but also for the at-risk populations.

This work contains the data and results of three quantifiable research studies in the field of chemical education. All three studies illustrate the positive effects of various classroom activities and interventions. These results are consistent with published studies showing how demonstrations and hands-on activities can greatly affect student performance. For example, at Missouri State University, researchers have shown that interactive demonstrations for mole ratios and limiting reagents can greatly improve student learning.[40]

In our first study a fun, effective, and low-cost classroom activity using LEGO bricks to model ionic formulas has been created and tested in an inner city high school classroom. Students who participated in this activity using manipulatives showed significantly higher post-test scores than did students who were taught by either a traditional lecture style or using a virtual game available online. This activity is an expansion to the set of previously published LEGO-based chemistry classroom activities. This activity gives a nice foundation in writing ionic formulas which teachers can use as an initial LEGO lab in a unit which follows with other more advanced LEGO labs in areas of stoichiometry,[5] reaction kinetics,[7] and design of advanced materials.[8-9]

The second study describes a computational chemistry lab module on molecular orbital theory that was implemented in an Honors General Chemistry course. Students who participated in the module in addition to attending a class lecture scored 22.7% higher on a 10 item multiple-choice post-test than students who attended lecture alone. While computational activities have been mostly introduced in upper-level chemistry classes[13-14] we have shown its effectiveness in General Chemistry. In 2004 Feller and co-workers described the creation of an extensive computational program at Wabash College

in Indiana. Their article entitled "A Program of Computational Chemistry Exercises for the First-Semester General Chemistry Course" is a description of the hardware and software used in the creation of their computational chemistry laboratory. Through a National Science Foundation grant, the authors were able to purchase computers and the software program PC Spartan Pro.[15] We believe that the effectiveness, low cost, and ease of administration of our experiment make it a valuable tool for chemistry teachers especially those at departments who already own ChemBio 3D Ultra. Many schools will be able to implement our module with no hardware or software purchases at all. While the introduction to General Chemistry students to computational chemistry is not entirely new, our study presents quantifiable results to show the effectiveness of our lab module on student learning. Additionally, our module can be a template to create further computational activities in more advanced courses such as organic, inorganic, and physical chemistry. Students who have already been introduced to computational chemistry as freshmen, will reap more benefits from similar activities in upper-level courses.

In the final study the goal of increasing percent success rates in CHEM 1100 has been obtained with the Reverse-Instruction students out-performing the standard lecture-based students with higher final exam scores and overall success in the class. As a result of this project, CHEM 1100 percent success rates more than doubled. This successful experience in CHEM 1100 transferred to a successful experience in CHEM 1110 where 73.7% of RI students who went on to take General Chemistry I were successful versus 48.4% from the ST (Standard Lecture-Based) classes. These results are some of the first quantitative data regarding the

effectiveness of Reverse-Instruction on student learning. While this methodology is currently being implemented in classrooms across the nation, the published articles relating to this topic are mostly qualitative in nature, relying on results of student surveys as their source of data for analysis.[29-35]

As this work illustrates, creative alternative methods of teaching can not only increase student success, but also can foster a new excitement in students taking a challenging science course. Not only have these methods increased student enjoyment of the courses, but also they make teaching more fun.

REFERENCES

(1) College Readiness Standards; http://www.act.org/standard/planact/science/p24.html (accessed May 2011).

(2) Mobile Chemistry Laboratory; Long, G.L. http://www.web.me.com/garylong/mcl/Welcome.html (accessed Oct 2010).

(3) Tro, N. J. Unit 6: Introductory Chemistry 4th Edition; Prentice Hall: 2011.
[4]Chimeno, J. S.; Wulfsberg, G. P.; Sanger, M. J.; Melton, T. J., *J. Chem. Educ.* **2006,** *83* (4), 651-654.

(5) Witzel, J. E. *J. Chem. Educ.* **2002,***79*(3), 352A.

(6) Carmen F., Mason D. *J. Chem. Educ.* **2008,** *85* (12), 1648A.

(7) Cloonan, C. A.; Nichol, C. A.; Hutchinson, J. S., *J. Chem. Educ.***2011,***88* (10), 1400-1403.

(8) Sharma, C. V. K., *J. Chem. Educ.* **2001,***78* (5), 617-622.

(9) Lohmeijer, G.G.; Schubert, U.S. *Polymer Chemistry.* **2003**, 41(10) 1413-1427.

(10) MindandHandAllianceandMITEdgertonCenter.LEGO® Chemistry.http://web.mit.edu/edgerton/outreach/ACT_LC.html (Accessed Dec. 2011)

(11) My Science Lessons Blog: A Collection of ideas, activities, and lessons for grades 5-8. http://mysciencelessons.wordpress.com/tag/atoms/(Accessed Dec. 2011).

(12) CambridgeSoft: Desktop Software. http://www.cambridgesoft.com/software/ChemBioOffice/ (Accessed Dec. 2010).

(13) Clauss, A. D.; Nelsen, S. F. *J. Chem. Educ.* **2009,** *86* (8), 955-958.

(14) Benatan, E.; Dene, J.; Eppley, H. J.; Geselbracht, M. J.; Jamieson, E. R.; Johnson, A. R.; Reisner, B. A.; Stewart, J. L.; Watson, L. A.; Williams, B. S., *J. Chem. Educ.* **2009,** *86* (6), 766-767.

(15) Feller, S. E.; Dallinger, R. F.; McKinney, P. C., *J. Chem. Educ.* **2004,** *81* (2), 283-287.

(16) Paselk, R. A.; Zoellner, R. W., *J. Chem. Educ.* **2002,** *79* (10), 1192-1194.

(17) Schmidt, M.W.; Baldridge, K.K.; Boatz, J.A.; Elbert, S.T.; Gordon, M.S.; Jensen, J.H.; Koseki, S.; Matsunaga, N. Nguyen, K.A.; Su, S.J.; Windus, T.L.; Dupuis, M.; Montgomery, J.A. *J. Comput. Chem.* **1993**, *14*, 1347-1363.

(18) Hoffmann, R. *J. Chem. Phys* **1963**, *39*, 1397-1412.

(19) Group II participated in the module after this study was completed.

(20) The University of Memphis Honors Living Learning Community Program. http://www.memphis.edu/reslife/livingcommunities/honors.php (Accessed Dec. 2010).

(21) Lilliefo, H. *J. Am. Stat. Assoc.* **1967,** *62* (318), 399-402; Shapiro, S.; Wilk, M. *Biometrika.* **1965,** *52*, 591-611; D'Agostino, R. B.; Belanger, A. *Am. Stat.* **1990,** *44* (4), 316-321.

(22) Ravid, R. Practical Statistics for Educators, 4th ed.; Rowman and Littlefield: Plymouth UK, **2011**.

(23) Mendenhall, W et al. *Introduction to Probability and Statistics*. Belmont, Ca: Thomson:Brooks/Cole, **2006.**

(24) Student Assessment of Learning Gains. http://salgsite.org (Accessed Jan. 2011).

(25) Seymour, E.; Daffinrud, S. M.; Wiese, D. J.; Hunter, A. B. G. *Abstracts of Papers of the American Chemical Society* **2000,** *219*, 480-CHED.

(26) College Readiness Standards; http://www.act.org/standard/planact/science/p24.html (accessed May 2011).

(27) Drelick, J.; Henry, Z.; Richard-Babbs, M.; Robertson-Honecker, J. *Journal of College Teaching* **2011,** *40* (4), 81.

(28) Drelick, J.; Henry, Z.; Richard-Babbs, M.; Robertson-Honecker, J. *Journal of College Teaching* **2011,** *40* (4), 81.

(29) Reverse Instruction: Dan Pink and Karl's "Fisch Flip; http://www.connectedprincipals.com/archives/1534 (accessed Aug 2011).

(30) Flip your classroom through reverse instruction; http://electriceducator.blogspot.com/2010/09/flip-your-classroom-through-reverse.html (accessed Aug 2011).

(31) Khan, S. Salman Kahn talk at TED 2011 [video webcast] http://www.khanacademy.org/talks-and-interviews/v/salman-khan-talk-at-ted-2011--from-ted-com (accessed April 2012).

(32) Lage, M. J.; Platt, G. J.; Treglia, M. *Journal of Economic Education.* **2000,** *31* (1), 30-43.

(33) Schaffhauser, Dian. The Backwards Class. http://thejournal.com/articles/2011/02/02/the-backwards-class.aspx (Accessed Apr. 2012).

(34) Hanford, E. Physicists Seek To Lose The Lecture As Teaching Tool. http://www.npr.org/2012/01/01/144550920/physicists-seek-to-lose-the-lecture-as-teaching-tool (Accessed Apr. 2012).

(35) Zappe, S.; Leicht, R.; Messner, J.; Litzinger, T.; Lee, H. *"Flipping" the Classroom to Explore Active Learning in a Large Undergraduate Course.* **2009,** American Society for Engineering Education.

(36) Student Assessment of Learning Gains. http://salgsite.org (Accessed Jan. 2011).

(37) Seymour, E.; Daffinrud, S. M.; Wiese, D. J.; Hunter, A. B. G. *Abstracts of Papers of the American Chemical Society* **2000,** *219*, 480-CHED.

(38) Ulriksen, L.; Madsen, L. M.; Holmegaard, H. T., *Studies in Science Education* **2010,** *46* (2), 209-244.

(39) Pascarella, E. T.; Pierson, C. T.; Wolniak, G. C.; Terenzini, P. T., *Journal of Higher Education* **2004,** *75* (3), 249-284.

(40) Wood, C.; Breyfogle, B., *Journal of Chemical Education* **2006,** *83* (5), 741-748.

APPENDIX I: Supplemental Information for Chapter 1

Student Activity Worksheet

A Building Block Activity in Writing Chemical Formulas of Ionic Compounds.

An important skill in chemistry is the ability to write chemical formulas. Cations (positive ions) and anions (negative ions) combine to form neutral compounds. In this activity you will need to refer to a table of ion charges to decide if an ion is trivalent (carries a charge of 3), divalent (carries a charge of 2), or monovalent (carries a charge of 1). Perhaps you will use plastic building blocks such as LEGO® bricks to model the formulas for ionic compounds.

You will need:

A set of LEGO Bricks for building: 3 blue 1x3's; 3 blue 1x2's; 3 blue 1x1's and likewise 3 red 1x3's; 3 red 1x2's, and 3 red 1x1's.

You may also complete the activity by downloading and installing LEGO Digital Designer at www.ldd.lego.com. You will have access to the same list of virtual bricks from above.

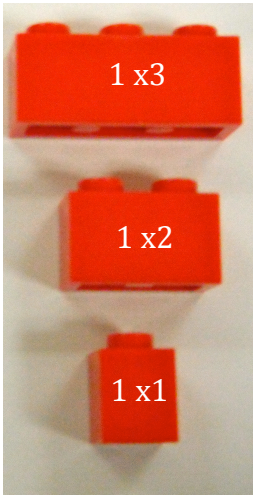


Figure I.1. Examples of different types of LEGO bricks shown in red.

Try This:

Step 1. Build LEGO models (use real LEGO bricks or virtual ones by installing LEGO Digital Designer at www.ldd.lego.com) of the chemical compounds listed in the first column of the data table according to the following rules:

1. Trivalent, divalent and monovalent ions are represented with 1 x 3, 1 x 2, and 1 x 1 bricks, respectively.
2. Cations are blue. Anions are red.
3. Neutral formula units are rectangular using the lowest whole number ratio of bricks. All blue bricks must be placed in a single row in the final rectangular product and likewise for the red bricks.
4. Example: Build a LEGO model of aluminum oxide.
   Al is a trivalent cation, Al^{3+}, and will be represented with a blue 1 x 3 brick. Oxide is a divalent anion, O^{2-}, and will be represented with a red 1 x 2 brick. In order to create a neutral (rectangular) formula unit, we need 2 blue 1 x 3's and 3 red 1 x 2 's. The formula is thus Al_2O_3. The subscripts in the formula are determined by how many of each type of brick is used. Write the

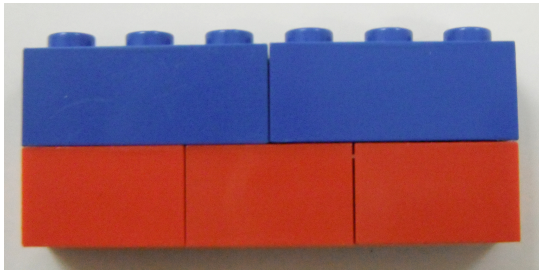


Figure I. 2. Finished model of Aluminum Oxide.

formula and the number of bricks used in the data table. This rectangular product (like an ionic formula) simply represents the lowest ratio of cations to anions needed for a neutral compound. Real compounds form complex crystal structures where this ratio is kept while the ions arrange themselves in different repeating patterns depending on the type of ions in compound.

Step 2. Now you will build models of the ionic compounds listed in the Data Table. For each compound you will identify the cation and anion. Next you will decide which type of blue brick represents the cation, and which type of red brick represents the anion based on the charge of the ion. These are the only two types of bricks you may use to build your compound. Build each compound in the data table recording the number of each color and type of brick you used, then write the formula for the compound. YOU MUST SHOW YOUR TEACHER EACH MODEL BEFORE MOVING ON TO THE NEXT.

Data Table								
			blue (cation)			red (anion)		
	Name	Formula	(1 x 1)	(1 x 2)	(1 x 3)	(1 x 1)	(1 x 2)	(1 x 3)
Ex.	aluminum oxide	Al_2O_3			2		3	
1	copper(II) chloride							
2	iron(III) sulfide							
3	silver(I) oxide							
4	potassium bromide							
5	ammonium sulfide							
6	calcium hydroxide							
7	aluminum sulfate							
8	ammonium nitrate							
9	sodium carbonate							
10	magnesium nitrate							

Questions

1. What is the cation to anion ratio in sodium carbonate?

2. How many hydrogen atoms are in ammonium sulfide?

3. When one molecule of iron sulfide decomposes into elemental iron atoms and sulfur atoms how many Fe atoms will be produced?

4. Is the Fe:S ratio different for iron(II) sulfide and iron(III) sulfide? Explain.

5. Build these compounds, sketch an image of the product (color code cations blue and anions red), and write the formula for the neutral compound: aluminum carbonate, sodium sulfide, ammonium phosphate, calcium nitride, and iron(II)oxide.

Information from the World Wide Web (accessed June 2011)

1. LEGO Home; http://www.lego.com/
2. LEGO Digital Designer; http/www.ldd.lego.com

Student Activity Worksheet Answers

A Building Block Activity in Writing Chemical Formulas of Ionic Compounds.

Data Table								
			blue (cation)			red (anion)		
	Name	Formula	(1 x 1)	(1 x 2)	(1 x 3)	(1 x 1)	(1 x 2)	(1 x 3)
Ex	aluminum oxide	Al_2O_3			2		3	
1	copper(II) chloride	$CuCl_2$		1		2		
2	iron(III) sulfide	Fe_2S_3			2		3	
3	silver (I) oxide	Ag_2O	2			1		
4	potassium bromide	KBr	1			1		
5	ammonium sulfide	$(NH_4)_2S$	2			1		
6	calcium hydroxide	$Ca(OH)_2$		1			2	
7	aluminum sulfate	$Al_2(SO_4)_3$			2		3	
8	ammonium nitrate	NH_4NO_3	1			1		
9	sodium carbonate	Na_2CO_3	2				1	
10	magnesium nitrate	$Mg(NO_3)_2$		1		2		

Questions

1. What is the cation to anion ratio in sodium carbonate? 2:1
2. How many hydrogen atoms are in ammonium sulfide? 8
3. When one molecule of iron (III) sulfide decomposes into elemental iron atoms and sulfur atoms how many Fe atoms will be produced?2 x Fe atoms
4. Is the Fe:S ratio different for iron(II) sulfide and iron(III) sulfide? Explain.Yes, for iron(III) sulfide the ratio is 2:3, but for iron(II) sulfide the ratio is 1:1.
5. Build these compounds, sketch an image of the product (color code cations blue and anions red), and write the formula for the neutral compound: aluminum carbonate, sodium sulfide, ammonium phosphate, calcium nitride, and iron(II)oxide.

Information from the World Wide Web (accessed June 2011)

- LEGO Home; http://www.lego.com/
- LEGO Digital Designer; http/www.ldd.lego.com

Post-test with answers

Ionic Formula POST-Test

____ 1. Cations are

a. negatively charged ions
b. neutral (no charge)
c. positively charged ions
d. never metal ions

____ 2. Which of the following ions is polyatomic?

a. oxide, O^{2-}
b. ammonium, NH_4^+
c. sodium, Na^+
d. chloride, Cl^-

____ 3. The cation to anion ratio in lithium bromide is

a. 1 : 1
b. 1 : 2
c. 2 : 3
d. 2 : 1

____ 4. Which of the following formulas of metal oxides is <u>incorrect</u>?

a. Al_2O_3 is aluminum oxide.
b. Fe_2O_3 is iron(III) oxide.
c. Na_2O is sodium oxide.
d. MgO_2 is magnesium oxide.

____ 5. Which of the following anions will combine with calcium cations (Ca^{2+}) to produce a compound with a 1:2 cation to anion ratio?

a. chloride
b. sulfide
c. carbonate
d. phosphate

____ 6. Which of the following is the correct formula for calcium sulfate?

a. Ca_2SO_4
b. $Ca_2(SO_4)_2$
c. $Ca_2(SO_4)_3$
d. $CaSO_4$

____ 7. How many magnesium atoms are contained in one formula unit of magnesium phosphate?

a. 1 b. 2 c. 3 d. 4

____ 8. Which of the following anions will combine with aluminum ion (Al^{3+}) to form a compound with a 1:1 cation to anion ratio?

a. chloride b. sulfide c. nitrate d. phosphate

____ 9. The correct formula for iron(III) nitrate is

a. $FeNO_3$ b. Fe_3NO_3 c. $Fe(NO_3)_3$ d. $Fe_2(NO_3)_3$

____ 10. The correct formula for ammonium sulfide is

a. NH_4S b. $NH_{42}S$ c. $(NH_4)_2S$ d. NH_4S_2

Post-Test Answers:

1. C
2. B
3. A
4. D
5. A
6. D
7. C
8. D
9. C
10. C

APPENDIX II: Supplemental Information for Chapter 2

Introductory Molecular Orbital Theory:
A General Chemistry Computational Lab
Using ChemBio3D

1. Pre-Lab Questions:

1.1. Draw Lewis dot structure(s) for H_2, N_2, CO and CO_3^{2-}. Assign formal charges and identify all resonance forms if applicable. Predict VSEPR shapes.

1.2. Look up the experimental carbon-oxygen bond lengths and angles in the carbonate ion.

1.3. What is the bond length for a carbon-oxygen (C-O) single bond?

1.4. What is the bond length for a carbon-oxygen (C=O) double bond?

1.5. Can a single Lewis dot structure represent the bonding in CO_3^{2-} ? Explain.

1.6. Draw the Lewis dot structure(s) for NO, nitric oxide. Explain any problems with this task.

2. Background Information

One method used by chemists to exchange ideas about the nature of the systems they study is through the use of models. Many models have been developed for describing molecules. One of the earliest chemical bonding models chemistry students study is that of valence bond theory. You utilized valence bond theory when you created the Lewis structures for your Pre-Lab assignment.

Valence bond theory or (the localized electron model) describes covalent bonding within the framework of pairs of electrons shared between atoms. Lewis structures are drawn and used to predict VSEPR geometries. The localized electron model has shortcomings, one of which is the assumption that electrons are restricted between (or shared between)

two atoms. For example, when describing the bonding in carbonate ion, CO_3^{2-}, three separate resonance structures must be drawn to fully describe the bonding. Experiment shows that in carbonate ion all three C-O bonds are the same length (1.30Å) and all O-C-O bond angles are 120 °. However, no single Lewis structure can be drawn to explain this bonding. The concept of resonance was developed to deal with this discrepancy between experiment and theory. In the case of carbonate ion, three Lewis dot structures must be used to represent the bonding.

A different and more modern model of bonding is that of molecular orbital theory in which electrons in a molecule are not treated as pairs which "belong to" a certain atom. Instead, molecular orbital theory combines atomic orbitals into whole molecule molecular orbitals. In this module we will investigate the differences between valence bond theory and molecular orbital theory using computational chemistry. More specifically, computations within ChemBio3D Ultra will be used to visualize and develop molecular orbital bonding schemes for small molecules.

The molecular orbitals generated in the modeling software package, ChemBio3D Ultra, are computed based on approximate solutions to the Schrödinger equation from quantum mechanics. The type of mathematical approximation varies with the computational method chosen.

$$\mathbf{H\Psi_{atomic} = E\Psi_{atomic}} \quad \text{Schrödinger Eqn.}$$

Heisenberg[1] and Schrödinger[2] developed mathematical descriptions of the wave properties of electrons in atoms. In the simplified version of the equation above, $\mathbf{\Psi}$ represents a mathematical function which describes the behavior of an electron in an atom. Atomic orbitals (s, p, d, f . . .) are discrete solutions to the Schrödinger equation. $\mathbf{\Psi}$ can represent electrons in molecules also. Approximate solutions to the equation are taken from linear combinations of atomic orbitals (LCAO), when the mathematical functions are added or subtracted. The molecular orbitals generated in this module are expressed mathematically as:

$$\mathbf{\Psi_{molecule} = c_1\Psi_1 + c_2\Psi_2}$$

Here $\mathbf{\Psi_{molecule}}$ is the molecular wave function, $\mathbf{\Psi_1}$ and $\mathbf{\Psi_2}$ are atomic wave functions, and c_1 and c_2 are coefficients which depend on the type of atomic orbitals being combined. Inherent in molecular orbital theory is the idea that electrons are not localized on specific atoms, but are spread out over the entire molecule. Molecular orbital theory offers a way of dealing with lone electrons (remember the difficulty you had in writing the Lewis dot structure for NO). Electrons do not necessarily exist in pairs.

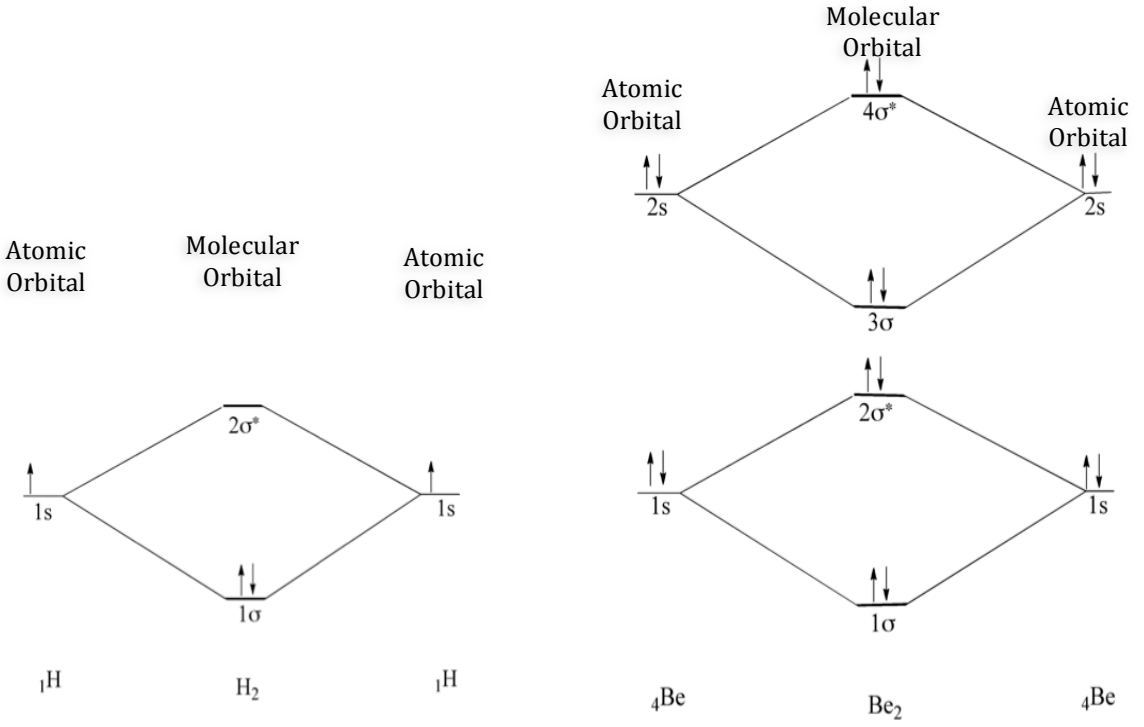
Just as two sound, light, or water waves can interact in two ways (constructively to

[1]Heisenberg, W. Über den anschulichen Inhalt der quantentheoretischen Kinematik und Mechanik. *Z. Phys.* **1927**, *43*, 172-198.

[2] Schrödinger, E. Über das Verhältnis der Heisenberg-Born-Jordanschen Quantenmechanik zu der meinen. *Ann. Phys*. **1926**, *79*, 734-756.

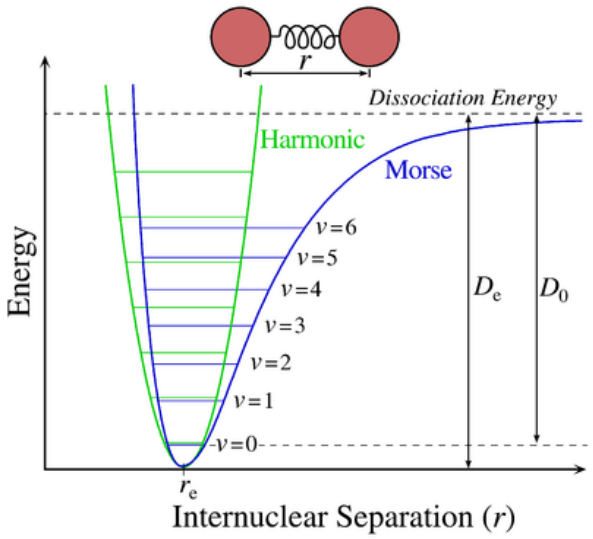
reinforce each other, or destructively to interfere with each other), so can orbital wave functions interact. In-phase (constructive) combinations yield what are called bonding orbitals (of lowered energy) while out-of-phase (destructive) combinations produce antibonding orbitals (of raised energy).

When the wave functions of atomic orbitals interact to form molecular orbitals, the total number of orbitals must be conserved. Two H atoms combining to form H_2 bring two 1s type atomic orbitals together. The diagram generated to represent the molecular orbitals formed must contain two orbitals (see **Figure II.1a).** Likewise molecular orbitals generated from two Be atoms (each with 1s and 2s atomic orbitals) interacting to form Be_2, must contain four total molecular orbitals as shown in **Figure II.1b**.



(a) H_2 **(b) Be_2**

Figure II.1. *Molecular orbital diagrams for H_2 and Be_2.*



.

Figure II.2. *Internuclear distance vs. energy for diatomics*

The **bond order** between the two H atoms is defined by the following formula:

(# bonding electrons – # antibonding electrons)/2

Thus the bond order for neutral H_2 is (2 – 0)/2 or a bond order of 1, which agrees with the single bond predicted in the Lewis dot structure. The bond order of Be_2 is (4 - 4)/2 or 0. A bond order of zero is in agreement with the fact that Be_2 is an unknown species.

A common task in computational chemistry is **energy (or geometry) optimization**. A geometry optimization algorithm performs successive energy calculations on a molecule, searching for the combination of bond distances and angles which compute as the lowest energy geometry. The energy-internuclear distance curve for a diatomic molecule given in **Figure II.2** illustrates how the energy of a molecule varies with bond distance.

In this activity, we will use a computational software package called GAMESS[3] (as implemented in ChemBio3D) to optimize the geometry for various small molecules.

[3] Schmidt, M.W.; Baldridge, K.K.; Boatz, J.A.; Elbert, S.T.; Gordon, M.S.; Jensen, J.H.; Koseki, S.; Matsunaga, N. Nguyen, K.A.; Su, S.J.; Windus, T.L.; Dupuis, M.; Montgomery, J.A.; *J. Comput. Chem.* **1993**, *14*, 1347-1363.

Hints for using ChemBio3D

Before you begin you will want to change one of the preferences in ChemBio3D.

Go to **File → Model Settings**. For **Model Display** make sure the choice for **Model Type** is Ball & Stick. For **Model Building** make sure to deselect "Correct Building Type," "Rectify," and "Apply Standard Measurements."

Click "**Set as Default**" at the bottom of the window before clicking "**Ok**"

3. Bonding in diatomics:

3.1. Use ChemBio3D to build the diatomic molecule H_2.

3.1.1. Begin by using the "**Build from Text**" function to build H_2 in the ChemBio3D window. On the toolbar, select the text box button and type H2 in the building window. An H_2 molecule will appear when you press enter.

3.1.2. Now move the mouse over the molecule to observe and record the H-H bond length.

3.1.3. Next you will minimize the energy of the molecule using GAMESS (The General Atomic and Molecular Electronic Structure System)which is a general **ab initio** quantum chemistry package. It computes wave functions using various methods.

a. Go to **Calculations → GAMESS Interface → Minimize (Energy/Geometry)**. The Minimize Energy dialog box appears with the Job & Theory tab displayed.

b. Use the default settings to run your computation. Check to make sure the default settings have not been changed from the following:

- **i.** Method: HF
- **ii.** Basis Set: 3-21G
- **iii.** Wave Function: R-Closed-Shell
- **iv.** Polarization: None
- **v.** Diffuse: None
- **vi.** Exponent: Pople
- **vii.** Opt. Algorithm: QA
- **viii.** Move Which: All atoms
- **ix.** Coord. System: Cartesian
- **x.** Select a Spin Multiplicity: 1
- **xi.** Net Charge: 0 (check mark Use Formal Charge)

c. Click Run.

d. Note the H-H bond distance after energy minimization.

Hints for using ChemBio3D

After geometry optimizations be sure to check the output panel to make sure the calculation completed normally. If it failed you may need to slightly adjust the geometry by moving an atom a little and then re-run the job. You may want to use the MM2 button on the tool bar to run a simple molecular mechanics optimization and then re-run the GAMESS calculation.

Also, remember to use your common sense. The geometry optimization algorithm may find a minimum which is not the global minimum. For example, f you are optimizing the geometry of carbonate ion and your result does not give a structure with 120° bond angles and three equal C-O bond lengths, the program has not found the correct minimum. You will need to change the geometry a little and try again.

3.1.4. Now you will perform an Extended Hückel [4] calculation to calculate the shape of the molecular orbitals for the molecule. [5]

a. Go to: **Calculations → Extended Hückel → Calculate Surfaces**.

b. An Extended Hückel calculation has been performed. The results of the calculation are stored with the model.

c. To view the computed molecular orbitals:

d. Go to **Surfaces →** choose **Calculation Result** and select **Extended Hückel**

e. Go to **Surfaces →** choose **Surface** and choose **Molecular Orbital.** You will most likely need to change the isocontour value.

f. To change the isocontour value, Go to **Surfaces → Isocontour →** and move the slider to a value of 0.070.

g. The default molecular orbital shown is the highest occupied molecular orbital or the HOMO. **Describe this orbital. Is it bonding or antibonding? Is the overlap constructive or destructive?**

h. To view the other molecular orbital(s) go to **Surfaces →** select **Molecular Orbital → LUMO** (Notice the energies of the orbitals are given in eV beside their designations. Record these energies). **Describe the LUMO. Is it bonding or**

[4] Hoffmann, R. *J. Chem. Phys* **1963**, *39*, 1397-1412.

antibonding? Is the overlap constructive or destructive?

i. The first complete molecular orbital diagram we will develop is that of the dihydrogen molecule, H_2 (see **Figure II.3**). The HOMO of H_2 results from σ-type bonding atomic orbital overlap. The LUMO of H_2 results from σ-type antibonding atomic orbital overlap. The 1s orbitals of each H atom interact to produce molecular orbitals. The left side of **Figure II.4** illustrates the formation of bonding and antibonding molecular orbitals between s orbitals. Notice how the two molecular electrons occupy the bonding type orbital which is lower in energy than the antibonding type orbital (Aufbau Principle).

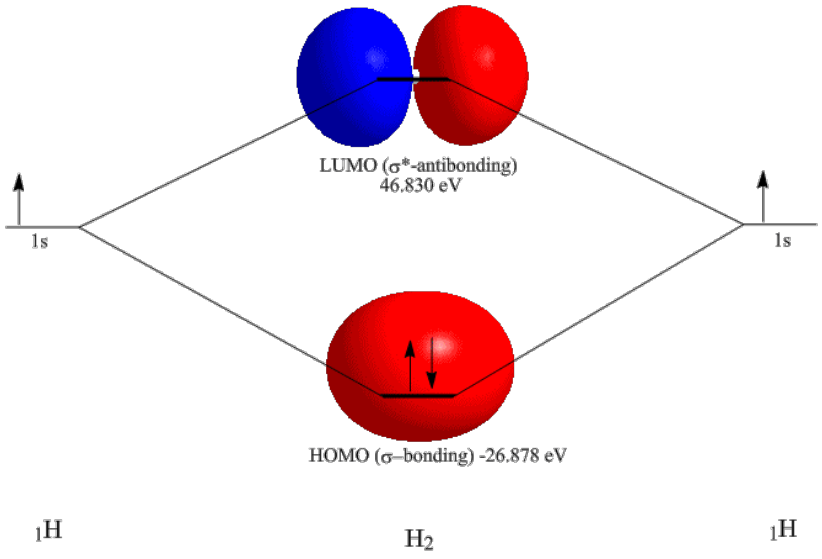


Figure II.3. *Computed molecular orbital diagram for H_2. Orbitals and energies generated in ChemBio3D using Extended Hückel theory.*

j. Now let's investigate the effect of adding an additional electron to dihydrogen to form H_2^-. Based on the molecular orbital diagram, what type of orbital must the additional electron occupy? Predict the effect this addition will have on the H-H bond length.

k. Remove the surfaces from the molecule. **Go to Surfaces → choose Surface → Remove All Surfaces.**

l. Now you will run a GAMESS calculation for the H_2^-. You will need to specify the charge and spin multiplicity in the input. Go to **Calculations → GAMESS Interface → Minimize (Energy/Geometry)**. The Minimize Energy dialog box appears with the Job & Theory tab displayed.

- **i.** Change the default settings to run your computation:
- **ii.** Method: HF
- **iii.** Basis Set: 3-21G
- **iv.** Wave Function: **RO-Restricted Open-Shell** (this setting is necessary because there is now an unpaired electron in the molecule)
- **v.** Polarization: None
- **vi.** Diffuse: None
- **vii.** Exponent: Pople
- **viii.** Opt. Algorithm: QA
- **ix.** Move Which: All atoms
- **x.** Coord. System: Cartesian
- **xi.** Select a Spin Multiplicity: 2
- **xii.** Net Charge: -1. Uncheck use formal charge.

Spin Multiplicity (M_S)

$$M_S = 2S + 1$$

S is the total orbital spin for all unpaired electrons. Here there is only one electron with a spin quantum number, m_s, of +½. So $S = m_s = +½$

$$M_S = 2S + 1 = 2(½) + 1$$

In this case, the number of unpaired electrons is 1, and M_S is 2. This is called a doublet. Zero unpaired electrons is called a singlet. Two unpaired electrons is of course a triplet.

- **xiii.** Note the H-H bond distance after energy minimization. Discuss how and why the bond length changed. What is the bond order for H_2^-? Can Valence Bond theory provide this same bonding description? Explain with the help of a molecular orbital diagram.

xiv. What happens to the H-H bond length when you add an additional electron to make H_2^{2-} ? Minimize the energy in GAMESS (Spin Multiplicity will be 1, charge will be -2). Discuss your observations in terms of a molecular orbital diagram. Go to **View → View Position → Fit to Window** to resize the view if the molecule goes beyond the viewing screen.

3.2. Use ChemBio3D to build dinitrogen, N_2.

3.2.1. Minimize the energy for N_2 in GAMESS. (Go to File →New to open a new window) Make sure you use the correct spin multiplicity and charge (M_s= 1, charge =0). Note the bond distance after minimization.

3.2.2. Now you will run an Extended Hückel calculation on this optimized geometry just as you did for dihydrogen.

a. Go to: **Calculations → Extended Hückel → Calculate Surfaces**.

b. An Extended Hückel calculation has been performed. The results of the calculation are stored with the model.

c. To view the computed molecular orbitals: Go to **Surfaces →** Choose **Calculation Result** and select **Extended Hückel**

d. An isocontour value of 0.020 is best.

e. Go to **Surfaces → Choose Surface** and choose **Molecular Orbital.** The orbitals generated are from the valence shell electrons only. In this case there are a 10 valence electrons in the molecule (5 valence electrons from each nitrogen atom) with 4 valence atomic orbitals ($2s^2p_x^1p_y^12p_z^1$) on each N atom combining to produce 8 molecular orbitals .

f. Go to **Surfaces →** Select and hover the mouse over **Molecular Orbital.** You will see 8 molecular orbitals (the 1s MO's are not shown) choices from ranging from HOMO-4 to LUMO+2. Notice the energy values in brackets for two sets of orbitals are the same. This means LUMO, LUMO+1 and HOMO-1, HOMO-2 are **degenerate** (equal energy)pairs.

g. Take a closer look at the HOMO-1 orbital and HOMO-2 orbitals. Rotate them around and examine them. These orbitals result from linear combinations of nitrogen p orbitals. The type of overlap is different from that seen in H_2. This overlap is called π-overlap which (in this case) results from the side-on overlap of two nitrogen p atomic orbitals. The right portion of **Figure II.4** illustrates π-type overlap of p atomic orbitals.

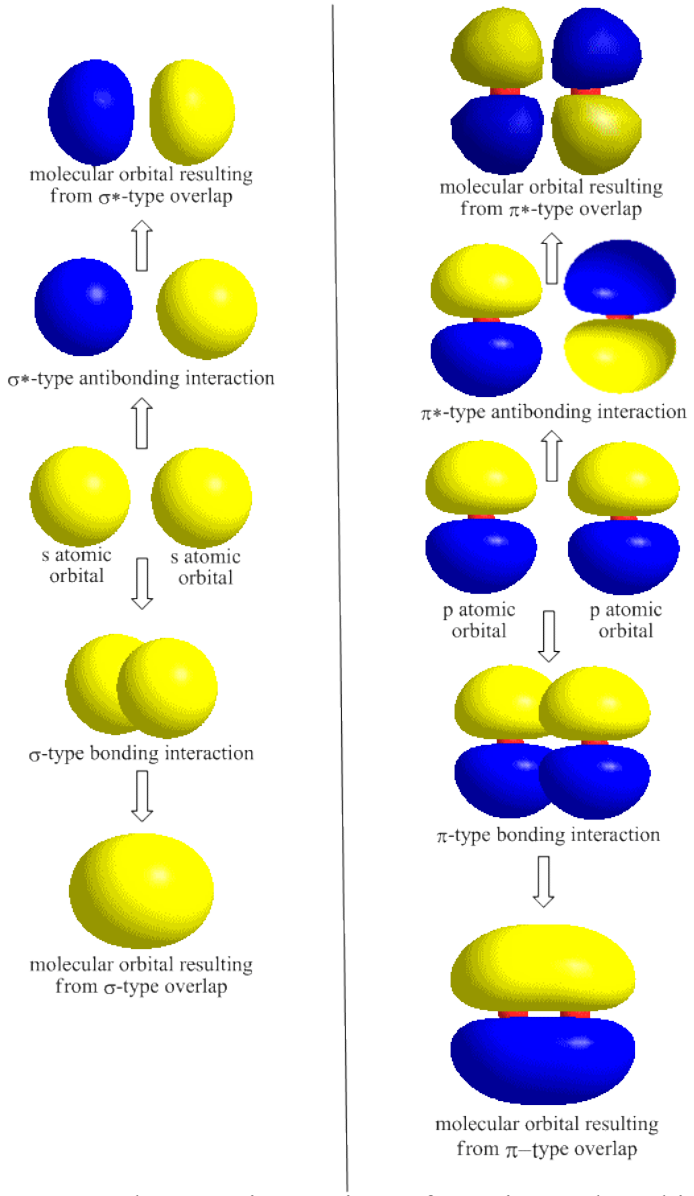


Figure II.4. σ and π- type interactions of atomic s and p orbitals

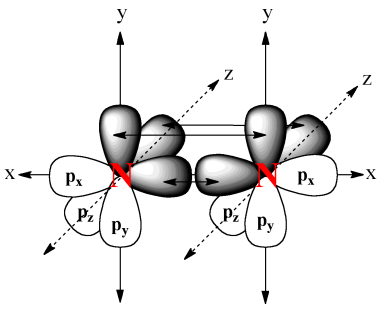


Figure II.5. π (p_z and p_y) and σ(p_x)-type overlap of nitrogen p orbitals in N_2.

When two atomic p-orbitals combine, two molecular π-type orbitals are formed. Addition of the atomic orbitals results in π-bonding, subtraction results in π-antibonding. A cartoon of the overlap between the p orbitals of the two nitrogen atoms of N_2 is given in **Figure II.5**. Two of the p orbitals (labeled p_z and p_y) overlap in a π fashion. The third p atomic orbitals labeled p_x overlap in a sigma (σ) fashion (only one lobe overlaps). Notice how overlap occurs DIRECTLY between the two atoms. The σ-type combinations of the p orbitals for N_2 are presented in the LUMO+2 and HOMO molecular orbitals. Examine these orbitals. Now examine all of the molecular orbitals and write in the labels for **Figure II.6** which correspond to the molecular orbitals formed from the nitrogen 2p and 2s atomic orbitals (for example write HOMO in the box). Include computed energies in eV. (Molecular orbitals formed from the 1s atomic orbitals are not computed).

h. What is the bond order for N_2?

i. Now run a GAMESS calculation for N_2^-**.** First remove the neutral N_2 surfaces by going to **Surfaces → Choose Calculation Result → Remove All Results.** (Remember to choose RO-Restricted Open-Shell, Change the Spin Multiplicity to 2, and the Net Charge to -1). How did the bond length change? Explain in terms of the molecular orbital diagram.

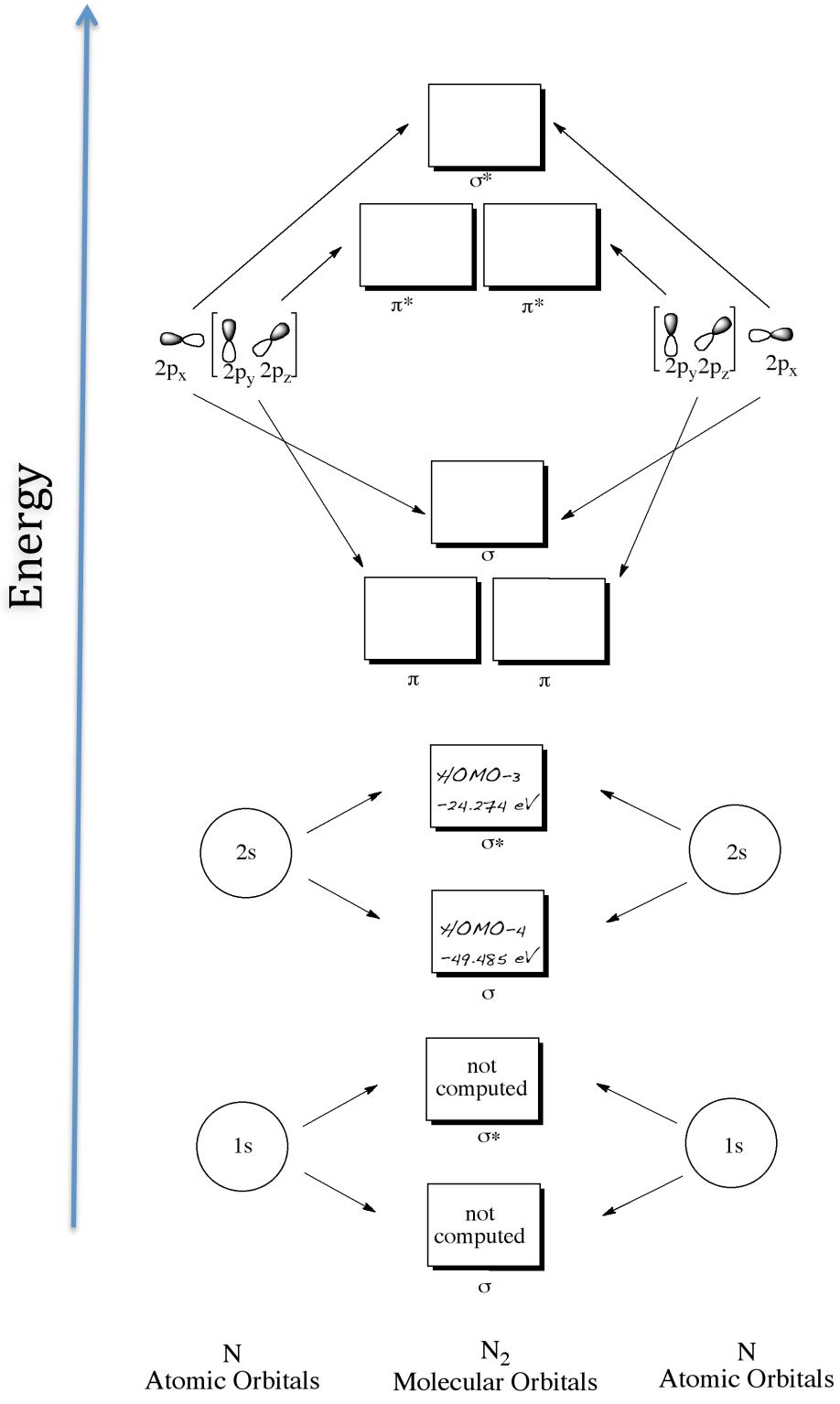


Figure II.6. Molecular Orbitals of Dinitrogen.

j. Run GAMESS (energy minimization) and Extended Hückel calculations for NO (neutral). The spin multiplicity will be 2 since it has one unpaired electron. Choose the **RO-Restricted Open-Shell** wavefunction. List the computed N-O bond length. Sketch the MO diagram (include energies of the orbitals from the Extended Hückel calculation). What is the bond order? How are the molecular orbital surfaces different in NO compared to the homonuclear diatomic N_2? Explain why you think this difference exists.

k. Compare and contrast the molecular orbital and valence bond (Lewis structure) theories for bonding in NO. Which theory best explains the fact that NO is a fairly stable molecule?

l. Minimize the energy of and NO^+ (ion) in GAMESS using the same methods (Think about what the spin multiplicity must be here). How did the bond length change compared to NO (neutral)?

4. Bonding in carbonate ion CO_3^{2-}:

4.1. Building the carbonate ion (CO_3^{2-}) structure in ChemBio3D:

4.1.1. Be sure Rectify and Correct Building Type are turned off in **File → Model Settings → Model Building**. Use the single bond drawing tool to sketch CO_3. Initially just draw all the atoms as carbons. Then select the **Build From Text** icon from the drawing toolbar. Click on the outer three atoms to change them to oxygen by typing **O** instead of **C**. Press enter each time. The outer atoms should become red.

4.1.2. Now use GAMESS to optimize the geometry. You will need to change the charge to -2. The spin multiplicity is 1. Note all three C-O bond distances. How do they compare to the experimental bond distances you looked up in your pre-lab? BE SURE THE ANSWER MAKES SENSE AND YOU HAVE FOUND THE GLOBAL MINIMUM (SEE HINTS ON PAGE 7).

4.1.3. Perform an Extended Hückel calculation on the optimized geometry. Generate the Molecuar Surfaces.

a. Go to: **Calculations → Extended Hückel → Calculate Surfaces**.

b. An Extended Hückel calculation has been performed. The results of the calculation are stored with the model.

c. To view the computed molecular orbitals:

d. Go to **Surfaces →** Choose **Calculation Result** and select **Extended Hückel**

e. Go to **Surfaces →** Choose **Surface** and choose **Molecular Orbital.**

YOU WILL NEED TO ADJUST THE ISOCONTOUR VALUE TO A REASONABLE VALUE TO BEST VISUALIZE THE MOLECULAR ORBITALS.

f. Which orbitals are degenerate pairs?

g. How would you describe the HOMO and HOMO-1 orbitals? Which atomic orbitals do they mainly represent?

h. How would you describe the HOMO-2 and HOMO-3 orbitals? Which atomic orbitals do they mainly represent?

i. How would you descibe HOMO-4 and HOMO-5 orbitals? Which atomic orbitals do they mainly represent?

j. The six orbitals discussed in g, h, and i have neither bonding nor antibonding character in great amounts. They are called non-bonding pairs. Is this description consistent with the Lewis structures from the pre-lab? Explain.

k. How would you describe HOMO-7? What atomic orbitals does it mainly combine? What type of overlap of these orbitals is present (Bonding? Antibonding? Sigma? Pi?)

l. How do you describe the LUMO +1? What atomic orbitals does it mainly combine? What type of overlap of these orbitals is present (Bonding? Antibonding? Sigma? Pi?)

Final Exercise

Now that you know how to perform geometry optimizations and generate molecular surfaces within ChemBio3D you will use computational chemistry to investigate the bonding in some other small molecules.

INVESTIGATION 1 IS REQUIRED. YOU MAY CHOOSE INVESTIGATION 2, 3, or 4.

You will need to save pictures of your molecules and orbitals generated in ChemBio3D and attach to into your document. To save a picture of what is displayed on the screen go to **File → Save As → Choose** TIFF (*.tif) and give the picture and appropriate name. Make sure to save the files to an external drive or email them to yourself. They will be deleted from the computer when you log out.

When generating your Molecular Surfaces, you may need to adjust your isocontour value.

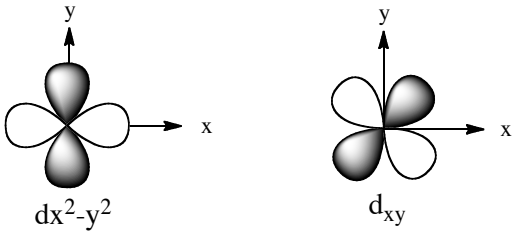
Viewing and analyzing the atomic components of molecular orbitals can be clarified by making your orbital surfaces translucent so you can see the molecule beneath (**Surfaces →Display Mode→ Transulcent**)

INVESTIGATION 1 (REQUIRED) You will describe the bonding in carbon monoxide.

Provide a valence molecular orbital diagram with images of the orbitals produced in ChemBio3D. Clearly label each molecular orbital as s, s*, p, or p* (The two molecular orbitals formed from overlap of the 1s atomic orbitals are not computed in the Extended Hückel calculation and they need not be shown in your MO diagram).

- How do the orbitals for CO compare to those for N_2?

- CO is described as both a σ-donor (HOMO) and a π-acceptor (LUMO) in terms of how it can interact with metal orbitals like the ones pictured. Use your results to explain what you think this statement means.



dx^2-y^2 d_{xy}

- Compare the C-O bond length in neutral CO to CO^+ and CO^-. (Remember the spin multiplicity for the ions will be 2, and since there is an unpaired electron you will need to run the GAMESS job using the **RO-Restricted Open-Shell** Wave Function. Don't forget to specify the correct charge. Explain the bond length changes in terms of the molecular orbital diagram.

- What is the bond order for all three molecules?

YOU MUST <u>CHOOSE ONE</u> OF THE FOLLOWING INVESTIGATIONS:

INVESTIGATION 2 (OPTIONAL) Minimize the energy of water in GAMESS .

- Describe the geometry of the water molecule.

- Perform an Extended Hückel calculation. Visualize the HOMO and HOMO-1. Save images of these three orbitals and print them out. Label these orbitals as bonding, antibonding, or non-bonding. Which electrons in the Lewis structure for water occupy these two orbitals?

- What happens to the structure of water when you remove an electron? Investigate by minimizing the energy of H_2O^+. Explain.

INVESTIGATION 3 (OPTIONAL) Compare and contrast the molecular shapes (bond lengths and angles) and bonding in NO_2, NO_2^- and NO_2^+.

- Minimize the energy of each molecule in GAMESS (Remember the spin multiplicity for neutral NO_2 will be 2, and since there is an unpaired electron you will need to run the GAMESS job using the RO-Restricted Open-Shell Wave Function.) How does the geometry change?

- Perform an Extended Hückel calculation for NO_2^-. Include a picture of the HOMO. How do you describe this orbital in terms

of overlap of atomic orbitals? Include a picture of the bonding orbital which shows delocalization of the π electrons amongst all three atoms.

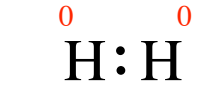
- How would the delocalization of the π electrons be represented with Lewis dot structures?

INVESTIGATION 4 (OPTIONAL) Minimize the energy of ammonia in GAMESS. Perform an Extended Hückel calculation and visualize the orbitals generated. You will need to change the isocontour value to 0.050.

- Include a picture of the HOMO. Describe it. Is the HOMO bonding, antibonding or non-bonding?

- Describe the other molecular orbitals.

1.1.

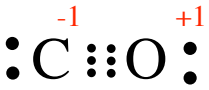


linear

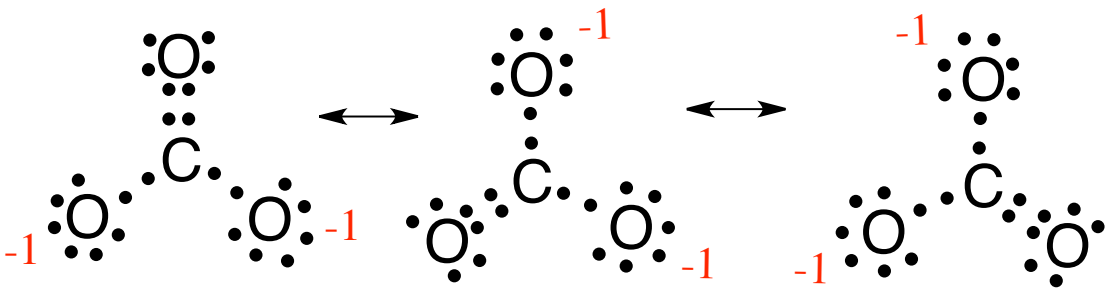
or

linear

linear



linear



trigonal planar

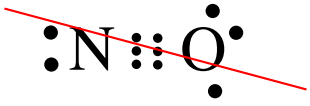
1.2 1.29Å, 120°

1.3 1.43 Å

1.4 1.22 Å

1.5 No, a single structure predicts different bond lengths.

1.6



has an unpaired electron

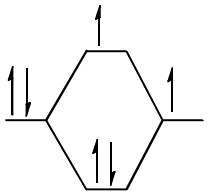
3.1.2. 0.704Å

3.1.3.d. 0.735Å

3.1.4.g. oval in shape -26.878 eV bonding (Constructive overlap, no nodes)

3.1.4.h. 46.878 eV bonding; separated flattened ovals; antibonding (empty/interference between atoms)

3.1.4.j. antibonding; bond length will increase

3.1.4.l.xii. 

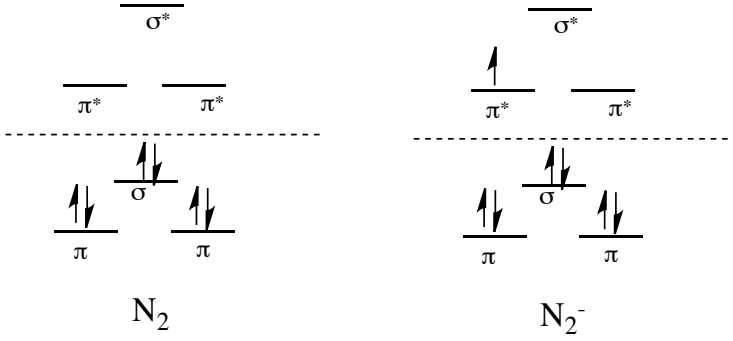
length = 1.496Å (longer due to lower bond order); bond order= ½; VBT

3.1.4.l.xiv. length increased to 7.558 Å. Bond order is zero. These atoms are essentially not bonded.

3.2.1. 1.083Å

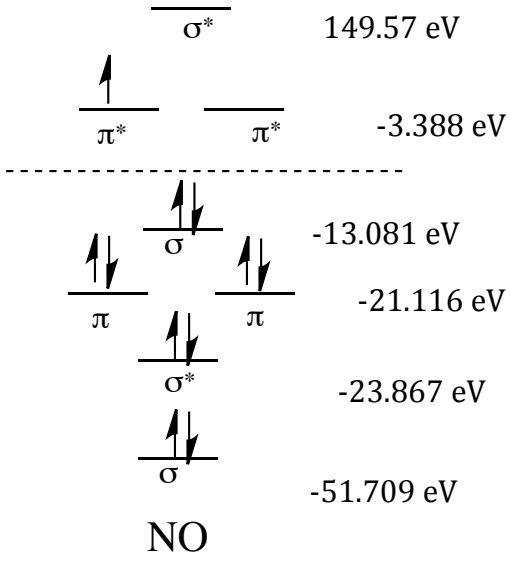
3.2.2.h. bond order = 3

3.2.2.i. increased from 1.083Å to 1.192Å; bond order changed from 3 to 2.5



N_2 N_2^-

3.2.2.j. length = 1.150Å; bond order = 2.5; Bonding orbitals are larger on O atom antibonding orbitals are larger on N atoms; both types were symmetrical in N_2



3.2.2.k. MO theory: bond order of 3 predicts greater stability. Valence bond theory shows a Lewis structure with a bond order of 2.

3.2.2.l. bond length = 1.047Å (shorter than NO which was 1.150Å)

suggests lone electron in NO was antibonding and bond order has increased

4.1.2. all 1.305Å very slightly longer than 1.29Å from pre-lab

4.1.3.f. HOMO -8 and HOMO-9; HOMO -4 and HOMO -5; HOMO -2 and HOMO -3; almost but not quite HOMO and HOMO -1

4.1.3.g. oxygen centered, bilobal shape, equal sizes; mainly oxygen p

4.1.3.h. large bilobal shape on 2 oxygens, smaller on 3rd; mainly oxygen p

4.1.3.i. oxygen-centered, bilobal shape with some O-O overlap; mainly oxygen p

4.1.3.j. Yes, Lewis structures had oxygen-centered lone pairs

4.1.3.k. molecular π orbital-bonding across all atoms but nodes directly between atoms; Carbon and oxygen p orbitals.

4.1.3.l. molecular π^* orbital-bonding across all atoms ; Carbon and oxygen p orbitals. combine destructively

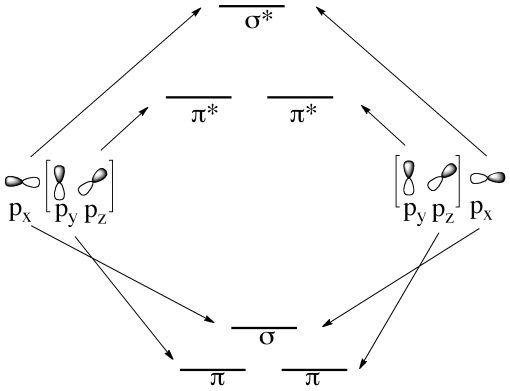
Introductory Molecular Orbital Theory Quiz

1) What type of overlap can possibly occur in the molecular orbitals formed from the combination of two p-type atomic orbitals?

a. σ and σ*
b. σ, σ*, and π
c. π and π*
d. σ, σ*, π, π*

2) Given the molecular orbital diagram, which orbitals are degenerate?

a. σ and σ*
b. the two π*
c. the two π
d. both b and c



3) What type of molecular orbitals are present in H_2 ?

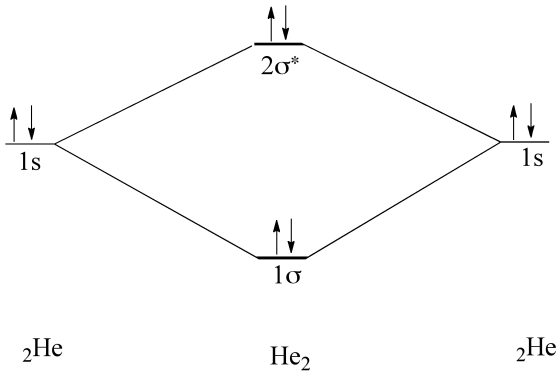
a. π antibonding
b. σ bonding
c. π bonding
d. both a and b

4) Bond order is calculated by

a. summing the number of electrons in bonding orbitals
b. (bonding electrons – antibonding electrons) * 2
c. (antibonding electrons – bonding electrons)/2
d. (bonding electrons – antibonding electrons)/2

5) Given the molecular orbital diagram to the right, calculate the bond order for He_2 .

a. 0
b. 2
c. 2.5
d. 1



6) Predict how the bond order will change upon removing an electron from He_2 to form the cation, He_2^+.

a. The bond order will remain the same.
b. The bond order will increase by 1.
c. The bond order will decrease by 0.5 .
d. The bond order will increase by 0.5 .

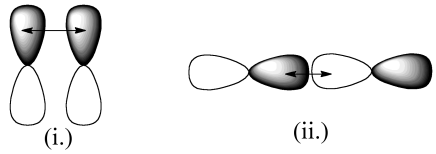
7) Which of the following will strengthen a bond between two atoms?

a. Removal of an electron from an antibonding orbital
b. Removal of an electron from a bonding orbital
c. Addition of an electron to an antibonding orbital
d. Transferring an electron from a bonding orbital to an antibonding orbital

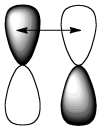
8) A complete molecular orbital diagram is generated for a homonuclear species, X_2. The total number of filled molecular orbitals (core and valence shell) generated is three. Which of the following would be X_2?"

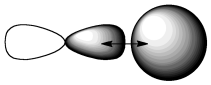
a. H_2
b. He_2
c. Li_2
d. B_2

9) Which of the following types of atomic orbital overlap is BOTH sigma type and bonding (σ) ?


(i.)

(ii.)


(iii.)


(iv.)

10) Which of the types of atomic orbital overlap in question 9 is pi (π)-type bonding overlap of p orbitals?

a. i. only
b. i. and ii. only
c. i. and iii. only
d. i., ii., and iii

Answers:

1. d
2. d
3. b
4. d
5. a
6. d
7. a
8. c
9. iv
10. a

SALG Student Evaluations of the Module: Free Response Comments

1.4 Please comment on HOW YOUR UNDERSTANDING OF MOLECULAR ORBITAL THEORY HAS CHANGED as a result of this experiment.

Responses

- "I understand the diagrams a great deal more now than when I first started out. Pi and Sigma bonds confused me a great deal in the beginning as well, but they make perfect sense now. "
- "To be honest, all new information that I learned using the ChemBio 3D software I learned through exploring away from the lab instructions."
- "never had an initial understanding"
- "more difficult to understand than most other chem topics, but lab coupled with lecture made it much more comprehensible"
- "Well-organized lab; explained things a little more clearly. Difficult time understanding the material but impressed with the clarity of the procedure."
- "I wish it was easier for me to recognize from a picture or a lewis structure if something had a sigma or a pi overlap-- that still confuses ne and I wish it didn't. On the other hand, I did learn about the differences in MO Theory and the VSEPR Theory. "
- "i understand more on bonding than i did by looking at them."
- "I didnt understand that certain bonds could exist before this lab."
- "I understand it some, as compared to not understanding at all."
- "It did help me see the orbitals and play around with them but i would have benefited more if mo theory was explained better in the class innstead of being thrown into it in the lab. The lab was good but since i didn't understand mo theory it was confusing."
- "I learned nothing because this was the first time that I was introduced to this."
- "very little. too little time spent on subject to be able to understand"
- "The experiment caused more confusion in my understanding of the Molecular Orbital theory. It was hard to use the program."
- "I really didn't learn anything from this experiment. The teaching was lackluster at best and there was little clear instruction given. The handout was unclear and the student was punished for not being able to clearly understand the murky instructions."
- "The visualization and hands on approach allowed more face-to-face time with the material."
- "I understand many of the diagrams well. I also understand the differences between the two theories very well."
- "I now slightly understand the theory but not very well."
- "For the most part, it was easier to visualize the type of bonding. Other than that, I didn't have much of an understanding before the experiment."
- "This lab was VERY helpful in understanding the difference between valence bond theory and molecular orbital theory. Before doing the lab, I don't think I really understood that they were two different theories. From this lab, I was able

to see how the orbits of the individual atoms of a molecule interacted to form the *molecular* orbits, which were spread out over the whole molecule. I was better able to connect this to the molecular orbital energy charts as well, as well as to see how anti-bonding orbitals looked like. It was also useful to be able to visualize unoccupied molecular orbitals, which I wouldn't normally have thought about."

- "I now fully understand the concept of pi and sigma bonding whereas before I did not. "
- "well it only slightly increased because i knew nothing of it before"
- "It helped me visualize the orbitals."

3.5 Please comment on how has this class CHANGED YOUR ATTITUDES toward the subject of Molecular Orbital Theory

Responses

- "It did nothing to change my attitude. "
- "I feel that the pace we moved at was too rapid for a student who lacks prior knowledge on MOT."
- "Made me think Chem is harder!"
- "realized that despite the mathematics and theory involved, still managable"
- "it honestly scared me. with a lot of hardwork and the same clearly-written material i could do it, but i'm terrified."
- "haha well it is still extremely complex for me. It's very hard to wrap your head around the idea, but it is semi "do-able" I just feel like it was too advanced for general chemistry. Sure the exposure was probably beneficial, but most of us had no clue what we were doing. That was extremely frustrating. "
- "i feel better about it because i could see what was happening."
- "It made me realize I dont want to do molecular orbital theory."
- "It has not."
- "I didn't understand the theory going into the lab so the lab just further confused me."
- "I do not enjoy it."
- "none"
- "It made me more confused in reference to molecular orbital theory. I learned almost everything from the lecture class."
- "All this did was confirm the fact that chemistry is not for me. The lab was very successful in completely destroying my self-confidence in the ability to learn and understand the molecular orbital theory. What little I knew was from lecture alone. This did nothing to expand my knowledge of anything."
- "Initial discouragement by not having adequate understanding of the theory to then attempt answering questions."
- "I prefer the Molecular Orbital Theory to the Valence Theory, but I find it much more complex. "
- "I still not sure about the theory but my attitude toward has not changed. "

- "It has made me realize that the Molecular Orbital Theory is quite complicated; yet, can be understand eventually."
- "This is the first time I have worked with a computational chemistry program, so it was very useful in becoming familiar with ChemBio 3D to get an idea of how to build molecular models. It was very helpful in helping me understand MO theory and visualize applications of its concepts. I am already a Chemistry major, so I will be taking many more chemistry classes, but after this lab, I feel more comfortable and confident about possibly taking a computational chemistry course."
- "I now understand it better but I think I was happier when I did not. "
- "i dont much enjoy molecular theory "

5.4 Please comment on how the INSTRUCTIONAL APPROACH to this class helped your learning

Responses

- "I learned it well enough. I answered all but one of the MO Theory questions correctly on my last exam."
- "The computer was a nice break away from the typical lecture style, however I believe that the majority of students did't fully understand what they were actually performing."
- "offer analogous explanations, or more examples rather than just pure theory"
- "more time was definitely necessary. the lab was given before the lesson on MO theory, and even after the lesson I was still confused. Lots more time, I could master it."
- "I truly wish we had been more prepared for this- nothing is more frustrating than writing a paper on something I do not completely grasp intellectually. I wish our teacher had introduced it a week before hand or something b/c the instruction during the lab was too quick. "
- "it was good i understood what i was supposed to do"
- "It allowed me to visualize different molecular bonds with ease."
- "The prelab was helpful but should have been more extensive."
- "We were thrown into this assignment."
- "slow down and be more through. class was rushed through just to get us to that part. had graded assignments over materiel we barley understood"
- "The instructional approach was not helpful at all. i was told two different things many times that changed my answers. The instruction was all over the place."
- "Although the instructors attempted to help a little, the ratio of lost students to mildly found instructors was too overwhelming for them to adequately provide any substantial assistance. "
- "The module we worked in class was helpful by starting with very basic models - but some of the more important concepts or the general objectives did not seem clear in comparison to the details."
- "The instruction explained quiet a bit of the material, but it did not help with

visualizing the models."

- "It did not"
- "The lab procedures should have been slower."
- "It was very helpful for our instructor to walk us through the beginning of the module, as well as having two weeks to complete the lab report, which was much more different from the other lab report we had to write for this class. It would have been a little more helpful to explain what we were seeing at first. That became the biggest challenge for me; it was a little hard to be able to identify whether I was looking at a sigma or pi bond, mainly because I didn't immediately make the connection that each atoms' orbitals all interact to form *molecular* orbitals."
- "I do not like to be told to figure things out by reading a manual or book, that's why I ask questions so that teachers can teach it to me."
- "the lesson helped for the first bit as she went through it with us but then when she cut the class loose to try it on their own everyone was lost"

6.3 Please comment on how the CLASS ACTIVITIES helped your learning

Responses

- "The class activities worked well enough."
- "Being able to build the 3D molecules in class with the teachers there to walk us through the process really helped, but the ChemBio lab didn't seem beneficial to me."
- "learned more from other students who grasped the theory better than myself"
- "the procedure was fantastic, because it was so clearly written and explained, and the instructions were fabulous. i could not understand what the answer was, but once i had it i could understand why. final lab report (personal investigations) was no help at all and made me feel like i learned it all wrong. "
- "seeing the orbitals made a difference- it was more of a struggle of working with the program- making sure no errors were made. "
- "i could see what to do on the assignment."
- "the lab report allowed me to articulate the concepts of the lab and helped me learn overall."
- "I was confused by the lab because it wasn't cover good in class."
- "The professors were stumped on some of the questions."
- "The small amount of information I was able to learn from the ChemBio3D Module was wasted when I attempted to write the lab report. The details of the report were never posted (as Ms. Ruddick said they would) so the grading was done unfairly because we did not know what was specifically supposed to be in the report. The actual module also did more to confuse me than help explain the Molecular Orbital Theory, this may be due to a lack of knowledge before going into the lab or the lack of explanation during the lab.

- “during the lab is when i started to understand the orbitals. but not the different types of orbitals”
- “My knowledge of the theory comes exclusively from what was taught in the lecture.”
- “The lab report was just a confusing mess of brain vomit thrown onto a page that showed more of the students ability to bullshit than the ability to write a report. I'm certain someone with no experience in chemistry could have walked in and attempted the lab and could have written the same level of report that someone who has taken the class could have. The grading of the report was so detrimental to students' self-esteem that it's a wonder no one had to go to therapy.”
- “The module helped speed up my understanding, but not to the point where I felt I could write 7 pages explaining it all. I didn't feel confident in that at all.”
- “The Pre-lab didn't help at all. The report was extremely difficult, but helped me understand better than the lecture. The Module was amazing for creating molecules.”
- “It forced me to read the material ”
- “Doing the lab report and ChemBio3D module was most helpful, as it really made us articulate the difference between valence theory and MO theory and make the connection using the molecules built in ChemBio3D. Although we were given an introduction to MO theory in lecture, it would have been more helpful to have a full class dedicated to it, including talk of the energy diagrams.”
- “It was much easier to comprehend when there is a 3D structure right in front of you, however while reviewing the material in a lab report I wasn't learning just remembering. ”
- “the lab reports were a lot of work for 1 hour of credit”

8.4 Please comment on how the RESOURCES in this lab helped your learning

Responses

- “Talking and having the lab instructor explain things (1 on 1 when necessary) worked explained things times better than any work given to me.”
- “The intro was not teaching, it was telling me info.”
- “once all of the ins and outs of the ChemBio 3D program were grasped, the theory was easy to comprehend”
- “Ms. Ruddick was a fantastic instructor and explained things well, but i feel like it was very simple and easy to understand with the H2 molecule, and then there was a wide chasm seperating that from everything else we "learned". It was good teaching, just not to a well-prepared class. i feel like if the class was better prepared then the lab wouldn't have been as difficult as it was.”
- “wish I had had better ones or more detailed instruction! especially when it came to using the program itself, and knowing what the changes meant. ”
- “i was able to use different things to learn how to do things”
- “It was slightly explained, but couldnt hold my attention long enough for me to learn it. Most of the learning was done on my own. ”

- "The lab packet helped but would have helped more if the class had given a good understanding."
- "It was hard to find resources while doing my postlab."
- "The resources used in the lab did not help at all. The presentations were confusing and not explained will. The packet made no sense becuase we only followed instructions and were not allowed to play around and figure out the controls of the program."
- "This is a topic that should be taught over a few days, not crammed down someone's throat in three hours. Honestly the sprint through the topic probably hurt more than it helped."
- "The presentations helped more than anything else. The lab helped a little, but was very confusing after the first 2 or 3 steps."
- "The lab packet and presentation by my lab instructor were most useful in my learning. My text book was very helpful when it came time to write the lab report. I also looked online to find energy diagrams for a few of the molecules discussed in the module (particularly CO, CO+ and CO- from investigation 1)."
- "The main resource that helped me in the lab was the lab instructor because she answered my questions easily. "
- "i thouhgt the program was cool but the lab was kind of lame"

10.5 Please comment on how the SUPPORT YOU RECEIVED FROM OTHERS helped your learning in this class

Responses

- "As I helped others, I basically taught myself."
- "interacting with other students during and after the lab was the greatest help"
- "as before-mentioned, good teaching just not to a well-prepared class."
- "my TA helped me a great deal- and so did the lab instructor. "
- "it was good if i did not understand it i could go to someone else for help."
- "We helped explain to each other the parts that we understood. without my freinds helping me i probably wouldve scoreed worse because i wouldnt have understood it otherwise."
- "The lab instructors and students help explain it in a better way."
- "We all failed as one unit."
- "We mostly pieced together what we were supposed to do from the different instructions that we were given."
- "If it wasn't for a few of my friends and I getting together and trying to trudge through the muck and mire of this desolate wasteland called a lab, I wouldn't have learned a thing. The lab instructors did very little to help during class do to the overwhelming amount of questions."
- "Everyone was too confused to really proceed well with the module - the lab instructors had to walk everyone thru each step or no progress was made. Working through it as a class would have been a more productive use of that time."

- “Working with others in the class helped me understand the material more than anything else. ”
- “If i didn't have the help of my peers I would not have passed. ”
- “The best support was when I was working one on one with the lab instructor.”
- “Our lab instructors, inside and outside of the class were most helpful in helping me learn through this lab. Dr. Petersen and Roger were very helpful in walking us through ChemBio3D in the lab, and I was very thankful to be able to meet with Kristie outside of class. I don't think I would have been able to really been successful in this lab had I not been able to meet with Kristie outside of class.”
- “Without the lab instructor and my self-designated partner I would have struggled much more in this lab.”
- “me getting help from classmates was very vital.”

APPENDIX III: Supplemental Information for Chapter 3

Table III.1. Post hoc comparisons using the Scheffe contrast among pairs of means for Fall 2011 sections. Reverse-Instruction sections (RI) are combined into one test group.

Group vs Group (Contrast)	*Test Statistics*	*p-level*
FALL 2011 Sections		
A & B(RI) vs ST-B	0.23832	0.9164
A & B(RI) vs ST-A	0.00433	0.99996
A & B(RI) vs ST-C	0.08962	0.98561
A & B(RI) vs ST-D	1.73272	0.14455
ST-B vs ST-A	0.19064	0.94307
ST-B vs ST-C	0.55593	0.69494
ST-B vs ST-D	0.73048	0.5722
ST-B vs ST-C	0.13456	0.96946
ST-A vs ST-D	1.65405	0.16256
ST-C vs ST-D	2.26607	0.06373

Table III.2. Post hoc comparisons using the Scheffe contrast among pairs of means for Spring 2012 sections. Reverse-Instruction sections (RI) are combined into one test group.

Group vs Group (Contrast)	*Test Statistics*	*p-level*
Spring 2012 Sections		
A & B(RI) vs ST-A	1.1309	0.34013
A & B(RI) vs ST-B	1.21815	0.30692
A & B(RI) vs ST-C	5.4333	0.00164
ST-A vs ST-B	0.01503	0.99747
ST-A vs ST-C	1.69898	0.17182
ST-B vs ST-C	1.23618	0.30043

Table III.3. Results of university SETE evaluation of teacher effectiveness. Fall 2011 CHEM 1100 sections.

	Graduate Student Sections			Faculty Sections		
	A (RI)	B (RI)	A(ST)	B-ST	C-ST	D-ST
1) I have become more competent because of this course.	4.00	3.88	4.20	3.53	3.96	3.07
2) I had an opportunity to ask questions in or outside of class.	4.31	4.06	4.57	4.10	4.40	4.00
3) The course was well organized.	3.94	3.69	4.40	3.93	3.76	3.53
4) The tests or other evaluation methods adequately assessed how well I learned the course material.	3.75	3.81	4.26	3.73	3.88	3.20
5) The instructor was enthusiastic when presenting course material.	4.06	4.00	4.34	3.00	4.40	3.60
6) The instructor was interested in teaching.	4.06	4.06	4.41	3.57	4.48	3.60
7)The instructor was concerned with whether the students learned the materials.	4.31	4.38	4.51	4.03	4.24	3.53
8) The instructor was knowledgeable about the subject.	4.00	4.13	4.49	4.38	4.48	4.20
9) In general, the instructor was an effective teacher.	3.94	3.93	4.26	3.60	4.08	2.93
MEAN RATING from 0-5	4.04	3.99	4.38	3.76	4.19	3.52

CHEM 1100 Reverse-Instruction Spring 2012. SALG Student Evaluations of the Course: Free Response Comments.

Results for Question: Please comment on HOW YOUR UNDERSTANDING OF THE SUBJECT HAS CHANGED as a result of this class.

Responses

- "I feel more confident with the material"
- "This helped me understand some of the math concepts better."
- "I understand more about why substances bind with others and how certain problems are solved "
- "I have learned more about chemistry then I did last prep chemistry"
- "For someone that did not take it in high school, I learned a great deal!"
- "Instructor Kristie Ruddick is a great teacher."
- "I have been able to remember what I learned in high school and learn more about Chemistry and this material helped me understand it very easily"
- "Before the relationships between some topics were not clear. After attend this class a lot of aspects became a lot more clear."
- "I understand a little bit more "
- "I knew absolutely nothing about chemistry before taking Dr. Ruddick's class. I had a horrible chemistry teacher in high school so I disliked the subject. But Ruddick opened my eyes to the entertainment of chemistry. "
- "I learned a lot of new things to prepare me for my next chemistry class "
- "The set up our teacher had helped my learning! "
- "It helped myself refresh on Chemistry from high school."
- "It has broadened all the way through."
- "I feel like I understand Chemistry a lot more and feel ready for the next step."
- "I wasn't familiar before with any of the work when I took the course my spring semester of my freshmen year, when I had Dr. XXXXX for my professor."
- "Professor Ruddick has made it more understandable through examples and patience with her class. Great Job! I wouldn't change my Prof if you paid me."
- "This is gotten better"
- "I've learned a lot."
- "Its been better"
- "I have a reasonable amount of knowledge from the course, but believe it could have been more extensive than it was."

Results for Question: Predicting products and amounts of products in chemical reactions

Responses

- "I didn't do so well in this section. The videos were a little hard to understand."
- "I obtained a good understanding of how much of certain products will react with others and under what circumstances."
- "More in class review on word chemistry"
- "na"
- "Some gain."
- "Makes a lot easier to learn and understand the material"
- "I've never been too good but she helps a lot "
- "Moderate gain"
- "I knew little about conversions but Ruddick has a set in stone way of setting the conversions up. Her consistency taught me a lot. "
- "I gained a lot "
- "At first it was a little difficult, but now I have a better understanding."
- "Very great "
- "I feel okay about predicting products."
- "The online homework and classwork definitely helped me enhance my skills when predicting products in a chemical reaction."
- "Still needs work but it's okay"
- "I'm better than I was."
- "I have a reasonable amount of knowledge from the course, but believe it could have been more extensive than it was."

Results for Question: Please comment on how has this class CHANGED YOUR ATTITUDES toward this subject.

Responses

- "More understandable than I thought."
- "I do plan on attending another chemistry class because this class made it easier but I still do not like working with people."
- "It has given me a deeper appreciation and understanding for chemistry. "
- "More positive towards chemistry"
- "It is still a challenging subject."
- "I will continue my studies in a teaching related field. "
- "This class has made me appreciate chemistry more and I look forward to take chemistry 1 and chemistry 2 later."
- "It made me more interested in chemistry"

- “This class changed my attitude in the way that I can like some aspects what I didn't like before”
- “I feel more comfortable talking to the teacher about it ”
- “I feel more confidant in it than I did before”
- “I didn't think chemistry would ever be fun or interesting. But it is. Probably the most interesting subject. ”
- “It has broken it down and made it easier to understand”
- “It has increased my attitude toward Chemistry. ”
- “It's helped me greatly.”
- “I feel ready for the next step in Chemistry.”
- “The class has built my confidence to want to continue my journey with chemistry.”
- “Chemistry is now easier”
- “Chemistry is not so scary to me now.”

Results for Question: What will you CARRY WITH YOU into other classes or other aspects of your life?

Responses

- “Understanding of chemical life and reactions”
- “I'm not quite sure.”
- “A stronger will to take responsibility for my own education.”
- “The basic of chemistry”
- “Not real sure...”
- “Problem solving with engineering”
- “Looking at situation in a different way”
- “If you believe and keep going you can reach everything, no matter how hard is it for you”
- “The ability to sit down and fully work out each problem and ask for help when needed ”
- “The formulas and equations”
- “CONVERSIONS!”
- “Everything I learned”
- “Decision making, and not second guessing myself.”
- “The way I approach, problems ”
- “Systematic reasoning in my approach to problems.”
- “I will carry everything I learned from this class. I mean everything I can remember!”
- “Nothing”
- “I can understand chemistry better.”

Results for Question: Please comment on how the INSTRUCTIONAL APPROACH to this class helped your learning.

Responses

- "I love the online material. Tremendously effective and helpful"
- "Watching the videos makes it easier to learn but people tend to forget to watch them. Keep having quizzes after them."
- "I had trouble with the technological aspect of the class but I have grown accustom to it and will be better prepared for it in the future."
- "I like the computer assignments really helped"
- "I personally need one on one because I didn't get it the first time."
- "I liked how we learned out of class and did problems in class"
- "It helped me to stay focused and organized on the work what we did in class"
- "I liked how she did the videos and then also taught over them! "
- "I wish we had more lectures on how to complete the lessons"
- "It did go a bit fast but Dr. Ruddick put everything in slow motion and rewind if we didn't understand."
- "I had to learn most by myself"
- "It gave me a much better understanding of the material."
- "Very hands on."
- "The instructor had videos for every lesson. "
- "The subject was very well organized so I didn't have any problem trying to keep up or understand unless I didn't study on my own."
- "I did not like that it was all online videos"
- "Great"

Results for Question: Please comment on how the CLASS ACTIVITIES helped your learning.

Responses

- "Repetition is king."
- "I really didn't participate in class actives like working with a partner but you should enforce that so others can seek help from their peers."
- "I am foremost a visual learner and I have always been able to obtain a better understanding of material through desiccations and examples of products."
- "I like being able to ask direct questions"
- "The homework reinforced what the concepts were."
- "The class was when we did the homework"
- "We did some good examples on the board, what helped me a lot to understand the material."
- "Many students asked questions that helped us all better understand "
- "It helped a lot more when we had class discussions"
- "I loved the whole watching the videos thing. I do wish there were a little bit more of lecture time but that's all. "

- “You had to do everything on your own”
- “They helped by being able to ask my teacher or one of my classmates for help.”
- “Greatly”
- “The instructor was open for any questions. ”
- “We had no class activities”
- “Good”

Results for Question: Please comment on how the GRADED ACTIVITIES AND TESTS helped your learning.

Responses

- “I just liked all the repetition and online work. Very helpful.”
- “The time period between the test are spaced really well and when extra credit is offered after the tests come back not satisfying is a plus. Also taking tests on ecourseware is much easier than paper. You have multiple choice which makes it easier than just writing something because you can make a good guess.”
- “Like the direct grades”
- “na”
- “You didn't go over enough of the tests after it was done.”
- “It showed how well I was progressing in class ”
- “The weekly tests helped me to keep learning the material.”
- “I really liked all the class work and homework online! ”
- “It helped having the tests on the computer”
- “The whole test review really helped for the upcoming tests. ”
- “It made me study more”
- “They showed what I needed to work on to better myself as a student.”
- “A lot.”
- “After every chapter or two, the class had a test.”
- “Well a couple of failed test made me realize that I need to study harder than usual.”
- “Made me study more”
- “They help me see where I was in the class”
- “Great”
- “Made me work harder”

Results for Question: Please comment on how the RESOURCES in this class helped your learning.

Responses

- “They were great and easy to use and maneuver”
- “being able to refer back to the text and videos for help is great. That way you can receive a better understanding.”
- “All you did was post videos you never actually worked problems in class and

allowed us to ask questions. ”

- “Like the videos and PowerPoint”
- “Worked good.”
- “The PowerPoint presentation helped me a lot in this class to understand the class material”
- “The online really helps ”
- “Mastering chemistry helped a lot”
- “I loved the online lectures but I do wish there were in class lectures as well. ”
- “IT just did”
- “The textbook and my teacher were very informative.”
- “A lot.”
- “The presentations from the instructor were great.”
- “The resources found online was very very helpful. I'd rather use the online sources than the book even though the book was additional help.”
- “The internet tool of mastering chemistry is priceless”
- “Online textbook and internet”
- “Great”
- “Basically guided me”

Results for Question: Please comment on how the SUPPORT YOU RECEIVED FROM OTHERS helped your learning in this class.

Responses

- “Professor Ruddick is awesome. Very helpful and always available for questions.”
- “When I did ask for help I received good help.”
- “The teacher was always available and great to work with”
- “I used the learning lab 75% of the time.”
- “Helped somewhat.”
- “Honestly, I don't have any experience about that. I didn't have support outside of class.”
- “Mrs. Ruddick was fantastic at working with her students until they understood what they needed to ”
- “It was good”
- “I had a great support team. The class was a whole and we'd work together to get done what needed to be done. ”
- “We helped each other”
- “I had support with a classmate that knew the material better than myself.”
- “Very much.”
- “The instructor was great help.”
- “My friends and I always tried working out with each other and at some points it was very helpful when we had the time to actually help each other.”
- “None”
- “Good”

Table III.4. SALG Student Evaluations of the Course: Ranked Items from 1-5. (1 being the lowest)

	Fall 2011 RI		Fall 2011 ST		Spring 2011 RI	
	Mean Rank	**# of Responses**	**Mean Rank**	**# of Responses**	**Mean Rank**	**# of Responses**
1. As a result of your work in this class, what GAINS DID YOU MAKE in your UNDERSTANDING of each of the following?						
1.1 The main concepts explored in this class	4	37	4.1	41	4.2	30
1.2 The relationships between the main concepts	3.9	37	4.0	41	4.2	30
1.3 The following concepts that have been explored in this class						
1.3.1 The math of chemistry	3.9	37	4.2	40	4.3	30
1.3.2 Chemical Reactions	4.1	37	4.2	40	4.1	30
2. As a result of your work in this class, what GAINS DID YOU MAKE in the following SKILLS?						
2.1 Writing chemical formulas	4.2	37	4.1	41	4.2	30
2.2 Performing unit conversions	3.7	37	4.1	41	4.2	30
2.3 Balancing chemical reactions	4.4	37	4.2	41	4.2	30
2.4 Predicting products from chemical reactions	4.1	37	3.9	41	3.7	30
2.5 Solving chemistry word problems	3.6	37	3.7	41	3.9	30
2.6 Apply math skills in chemistry	3.9	37	3.9	41	4.1	29

3. As a result of your work in this class, what GAINS DID YOU MAKE in the following?						
3.1 Enthusiasm for chemistry	3.2	36	3.2	40	3.5	30
3.2 Interest in taking or planning to take additional classes in chemistry	3.3	36	3.3	39	3.3	29
3.3 Confidence that you understand the material	3.6	37	3.7	41	3.9	30
3.4 Your comfort level in working with complex ideas in science	3.5	37	3.5	41	3.8	29
3.5 Your willingness to seek help from others (teacher, peers, TA) when working on academic problems	3.7	36	4.2	40	3.9	29
4. As a result of your work in this class, what GAINS DID YOU MAKE in INTEGRATING the following?						
4.1 Connecting key class ideas with other knowledge	3.4	37	3.5	39	4.0	29
4.2 Applying what I learned in this class in other situations	3.1	36	3.3	39	3.7	29
4.3 Using systematic reasoning in my approach to problems	3.3	37	3.4	40	3.8	29
4.4 Using a critical approach to information and arguments I encounter in daily life	3.1	37	3.2	39	3.7	29
5. HOW MUCH did the following aspects of the class HELP YOUR LEARNING?						

5.1 The instructional approach taken in this class	3.6	37	4.0	41	3.9	30
5.2 How the class topics, activities, reading and assignments fit together	3.3	37	4.1	41	3.9	30
5.3 The pace of the class	3.8	37	4.0	41	3.7	30
6. HOW MUCH did each of the following aspects of the class HELP YOUR LEARNING?						
6.1 Attending lectures	3.1	36	4.1	40	3.8	30
6.2 Participating in discussions during class	3.4	37	3.8	41	3.7	29
7. HOW MUCH did each of the following aspects of the class HELP YOUR LEARNING?						
7.1 Graded assignments (overall) in this class	3.7	37	4.0	41	4.0	30
7.3 The number and spacing of tests	3.6	37	3.9	41	4.0	30
7.4 The fit between class content and tests	3.5	36	3.9	41	4.0	30
7.5 The feedback on my work received after tests or assignments	3.5	37	3.5	39	3.7	30
8. HOW MUCH did each of the following aspects of the class HELP YOUR LEARNING?						
8.1 The textbook	3.1	37	3.1	40	3.9	29
8.2 Other reading materials						
8.2.1 Reading material	3.2	3	3.2	33	3.7	27
8.2.2 MasteringChemistry tutorials	3.5	37	3.6	39	4.0	30

8.3 Online notes or presentations posted by instructor	3.9	37	3.9	41	4.5	30
9. HOW MUCH did each of the following aspects of the class HELP YOUR LEARNING?						
9.1 Explanation given by instructor of how to learn or study the materials	3.5	34	4.0	41	4.1	30
10. HOW MUCH did each of the following aspects of the class HELP YOUR LEARNING?						
10.1 Interacting with the instructor during class	3.7	37	3.7	40	4.1	30
10.2 Interacting with the instructor during office hours	3.5	27	3.2	28	3.7	24
10.3 Working with teaching assistants outside of class (e.g., recitation, office hours)	2.9	24	2.9	27	3.8	25
10.4 Working with peers outside of class (e.g., study groups)	3.1	31	3.5	32	3.7	27
OVERALL AVG Ranking	3.56		3.73		3.92	